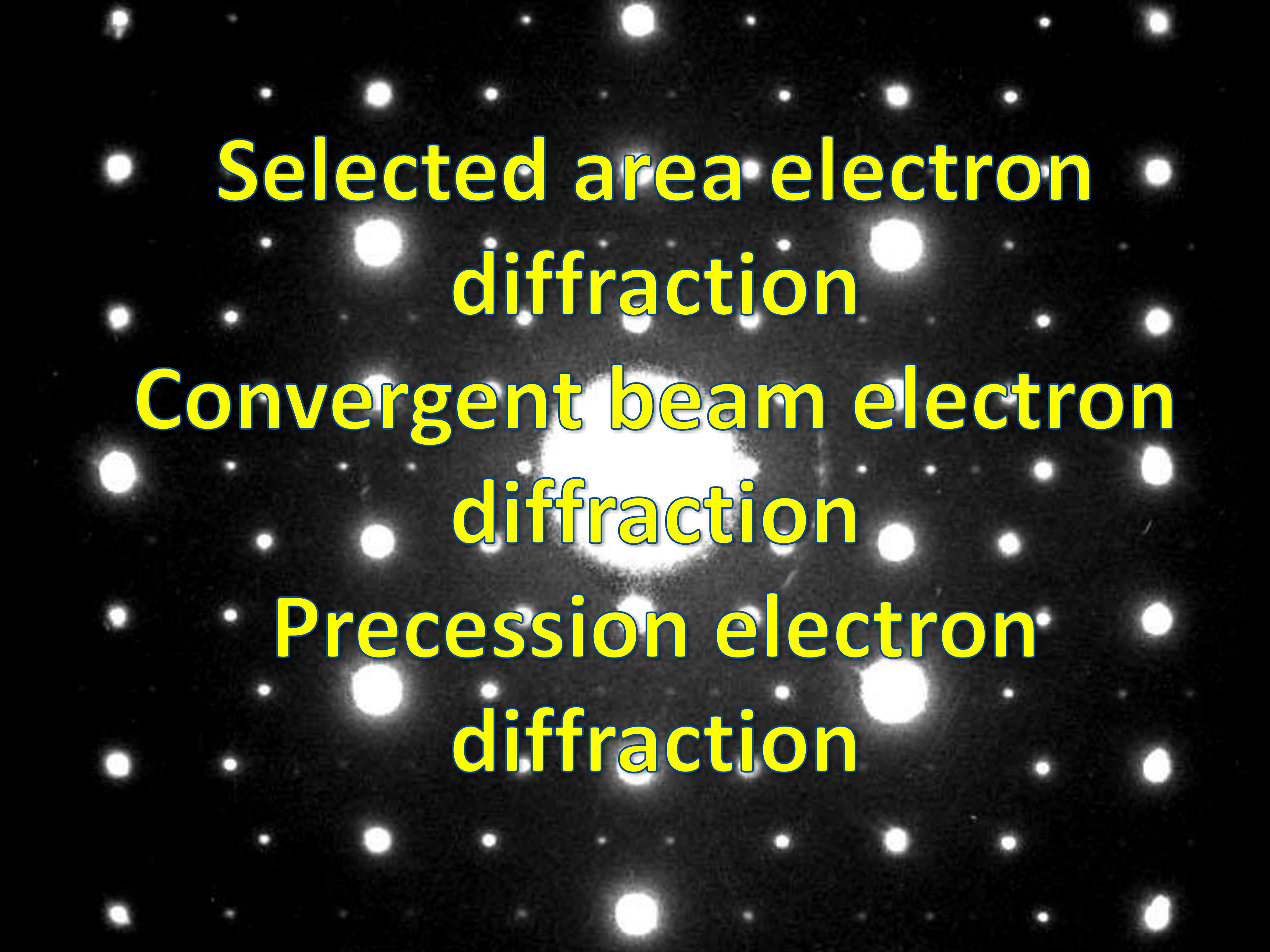


Selected area electron diffraction
Convergent beam electron diffraction
Precession electron diffraction

Purpose of this lecture

At the end of this lecture, you should be able to

1) index SAED patterns if the cell parameters are known
2) know how to determine unknown cell parameters from SAED patterns
3) determine the possible space groups from SAED patterns
4) determine possible point groups from CBED patterns
5) solve a simple structure ab initio from PED patterns

Example materials used in this lecture

Aluminum

Rutile-type SnO_2

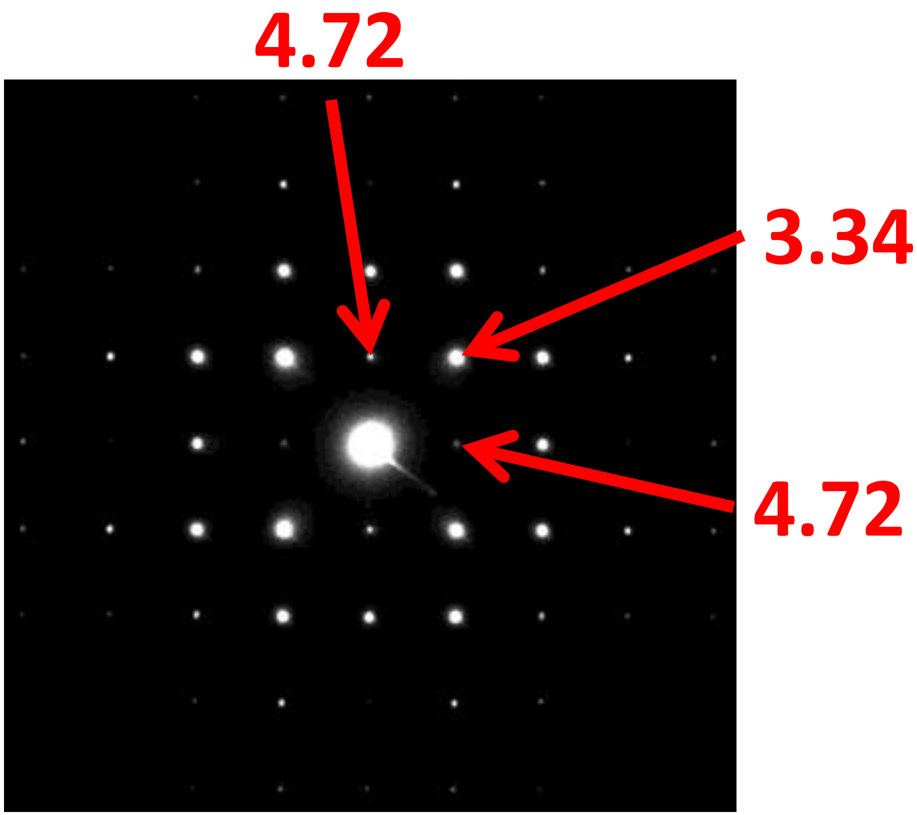
Slides are on http://www.slideshare.net/johader

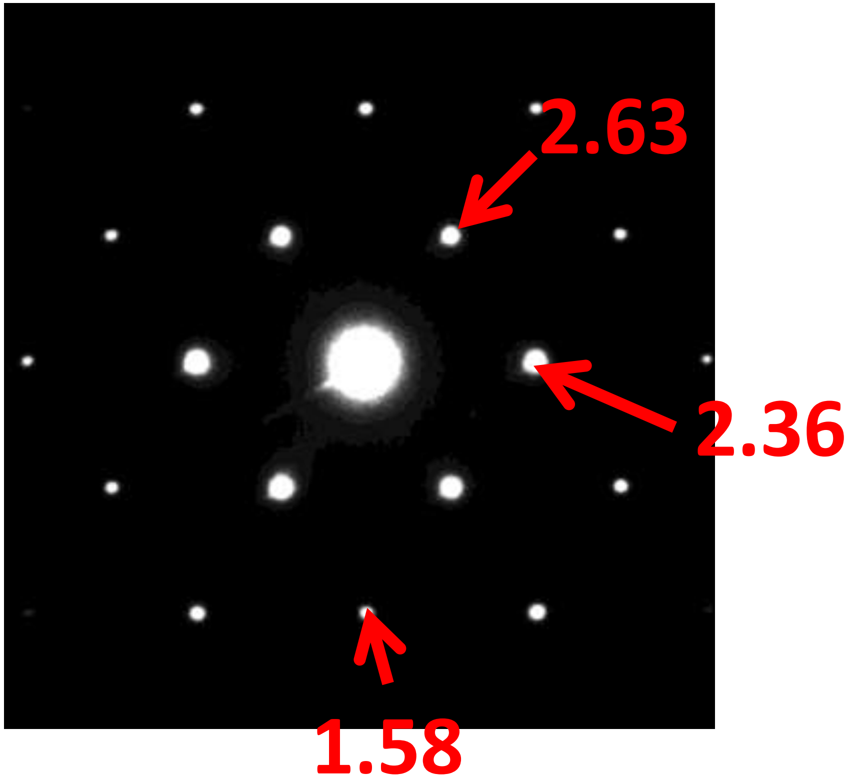
The pages with the ED for the exercises can be found at the end of this ppt.

1. Selected area electron diffraction (SAED)

Example 1: a known material, e.g. SnO_2

Tetragonal, a=b= 4.72 Å, c=3.16 Å





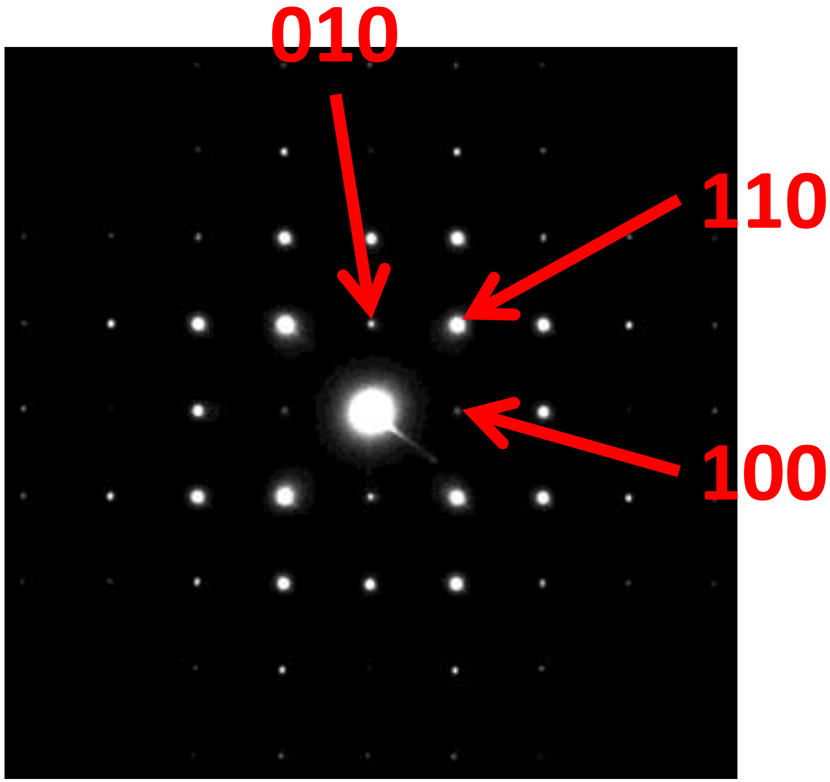
List of hkl – d

Powdercell

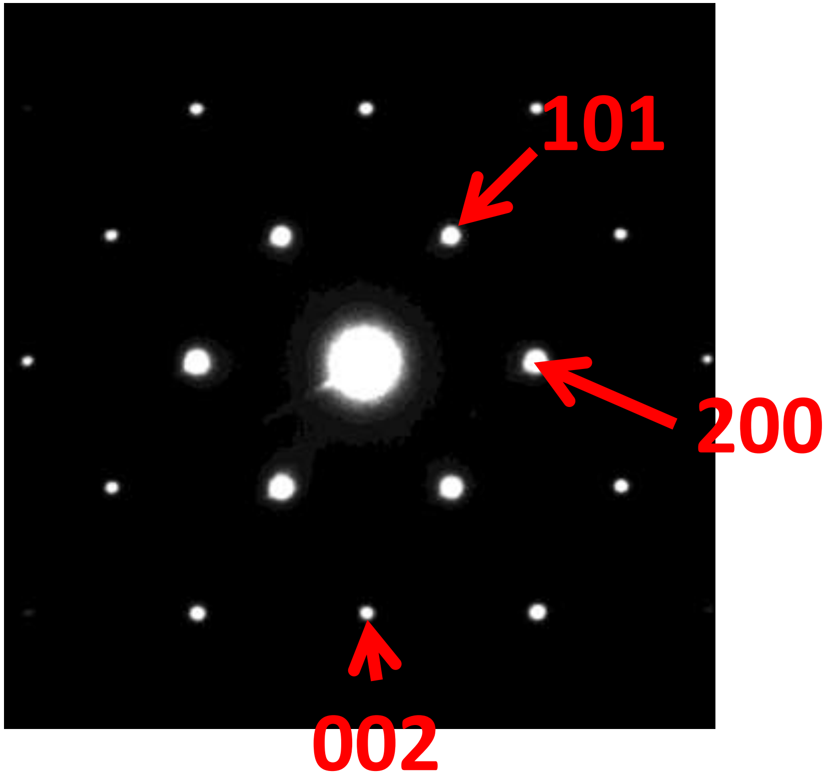
Input:
P42/mnm
a=b=4.72 Å
c= 3.17 Å

H	K	L	2Theta	d/Å
1	1	0	26.688	3.33754
1	0	1	34.041	2.63158
2	0	0	38.101	2.36000
1	1	1	39.161	2.29848
2	1	0	42.806	2.11085
2	1	1	52.007	1.75697
2	2	0	54.980	1.66877
0	0	2	58.155	1.58500
3	1	0	62.139	1.49260
2	2	1	62.886	1.47666
1	1	2	65.097	1.43175
3	0	1	66.266	1.40930
3	1	1	69.560	1.35039

Determine the zone-axis



[001]



[010]

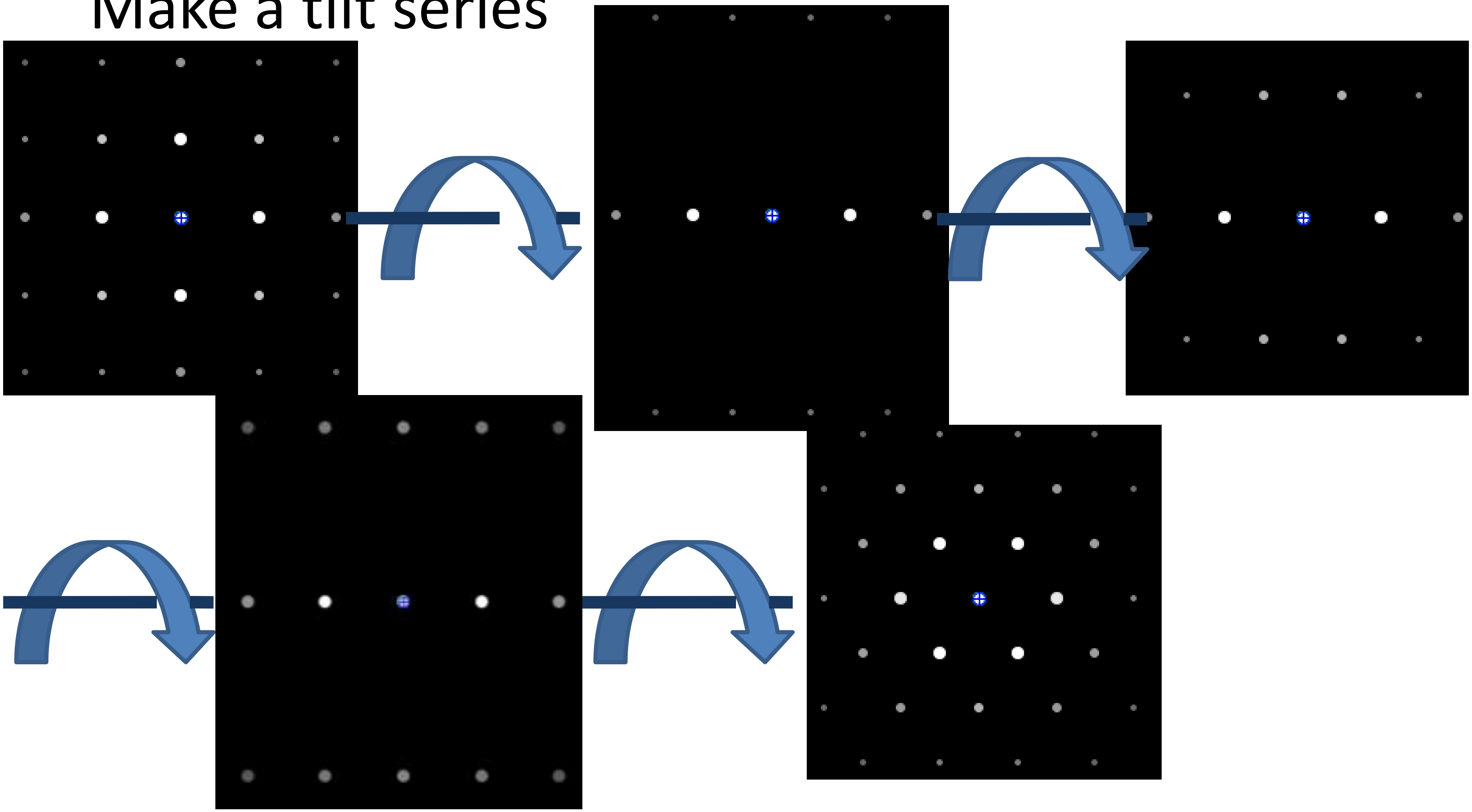
If cell parameters/material unknown

Shortest vectors, high symmetry, ...

best during TEM experiment

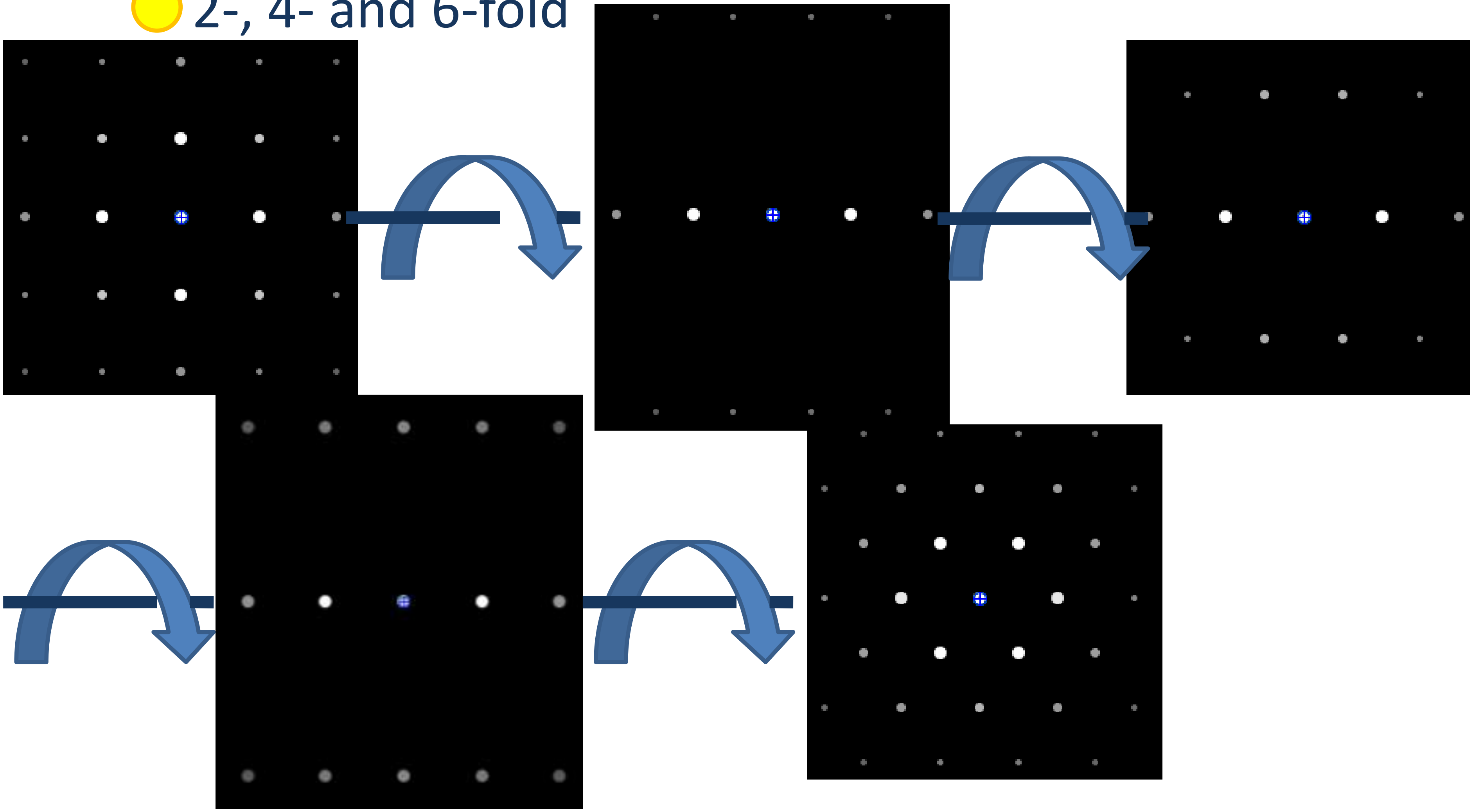
Starting from nothing: aluminum
First determine the cell parameters

Make a tilt series



Do you recognize any typical symmetry?

- Only 2-fold
- 2- and 4-fold
- 2-, 4- and 6-fold



Do you recognize any typical symmetry?

- Only 2-fold
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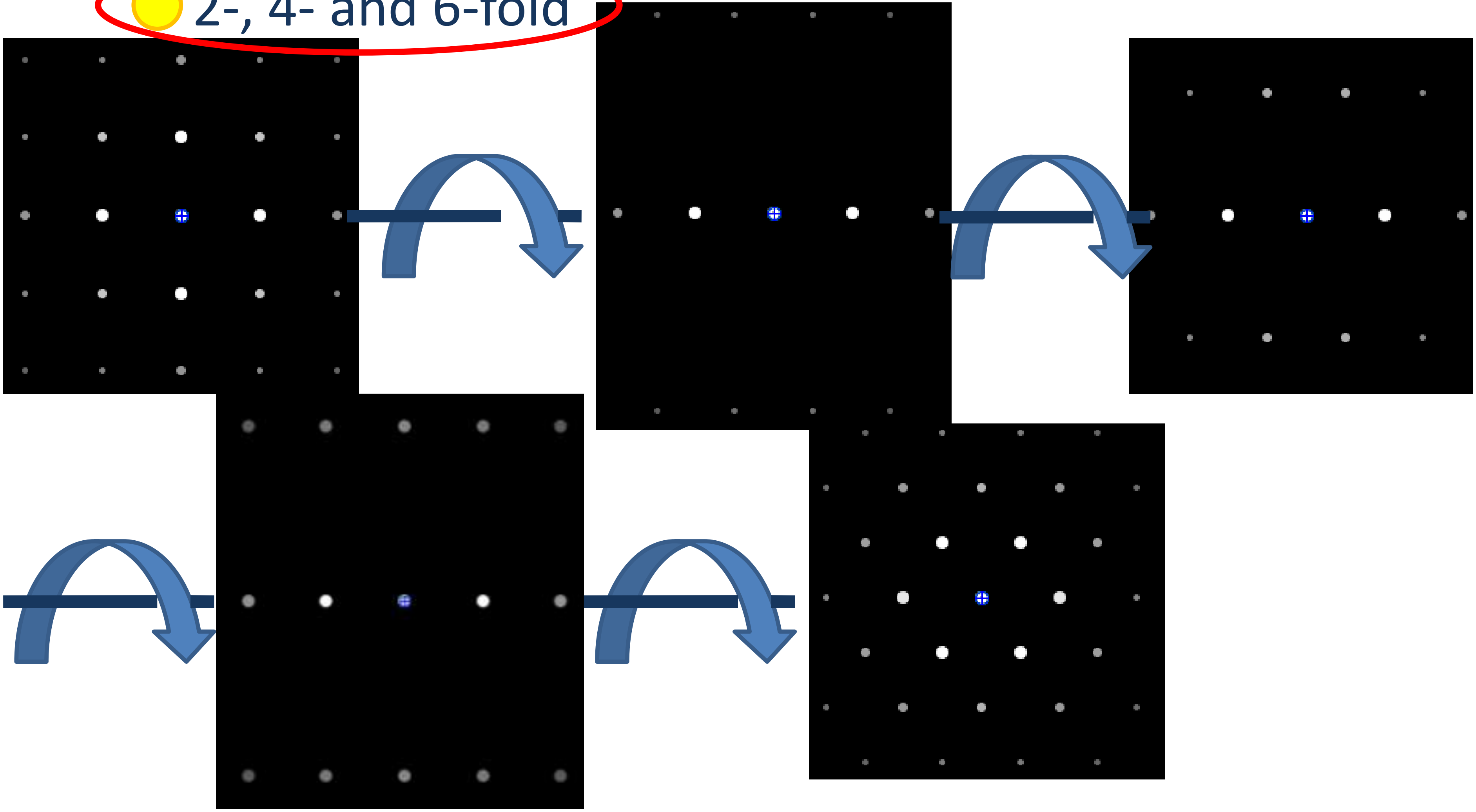
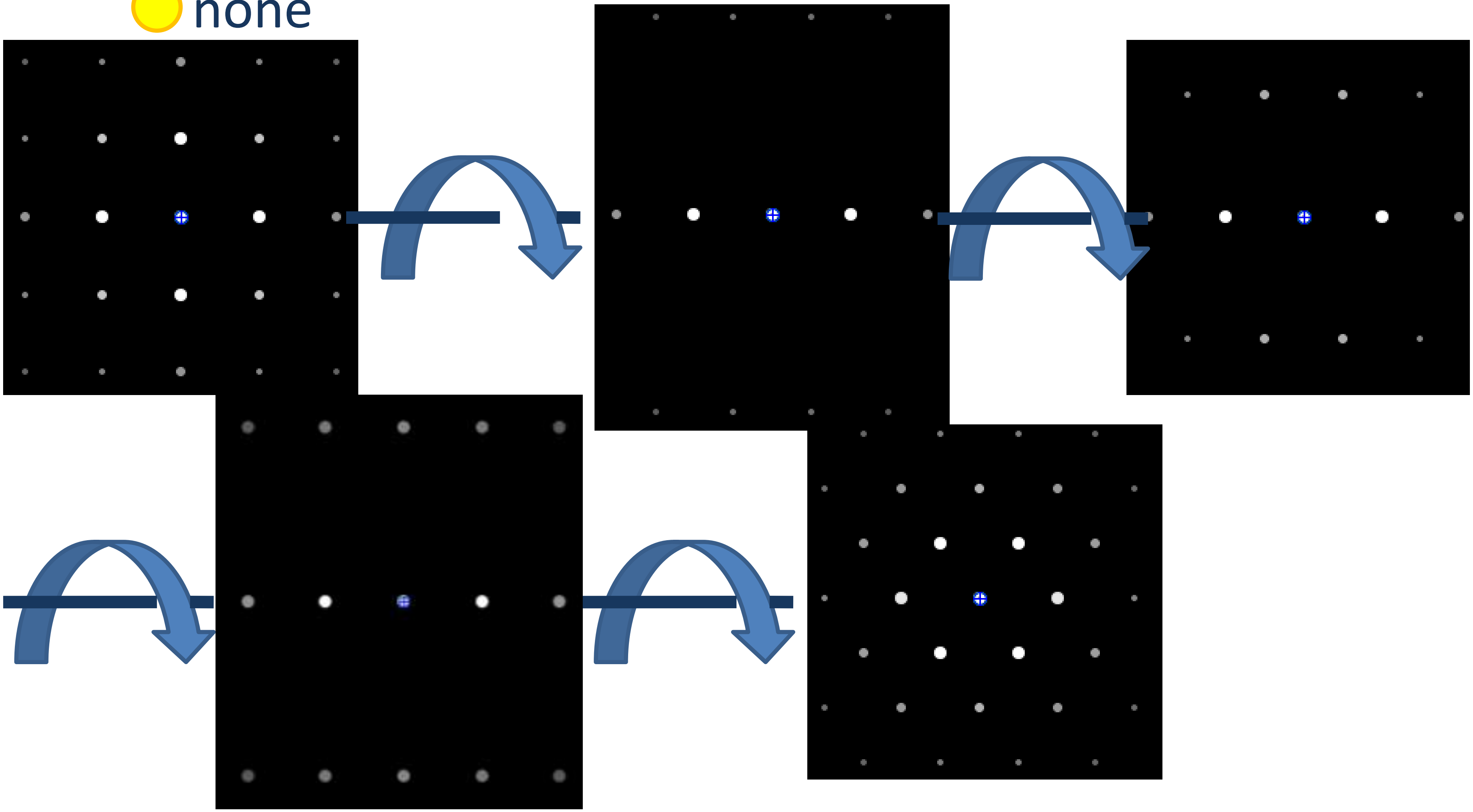


What crystal class has both 4-fold and 6-fold axes?

- cubic
- hexagonal
- none



What crystal class has both 4-fold and 6-fold axes?

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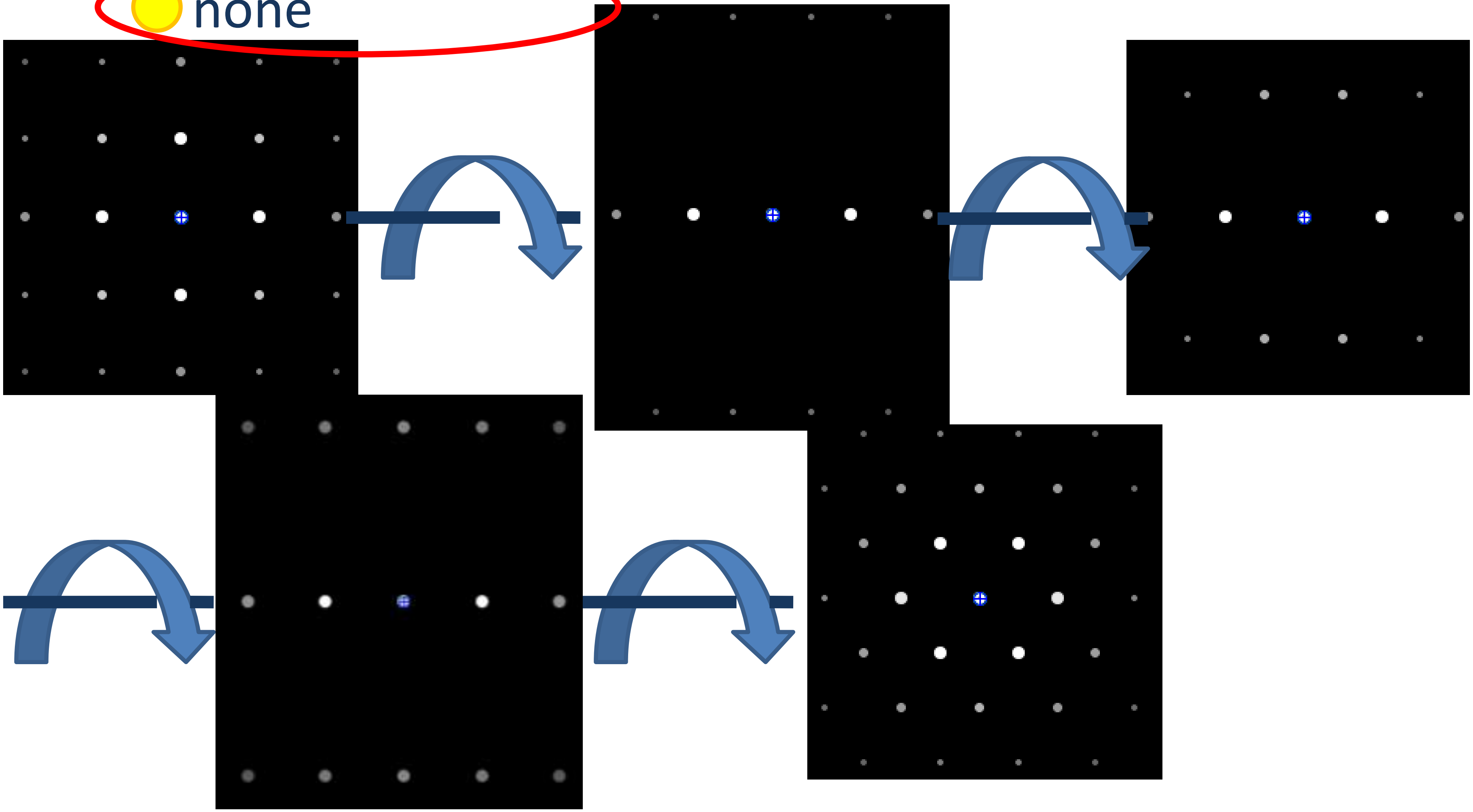
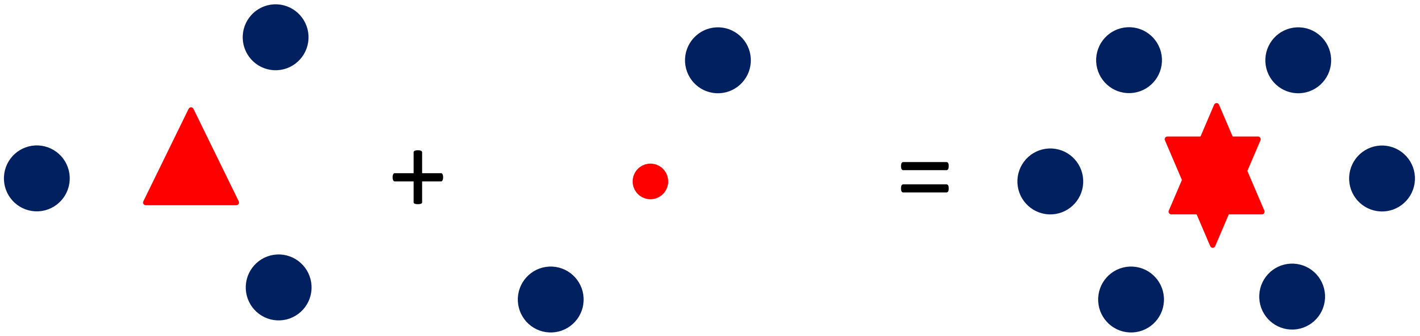
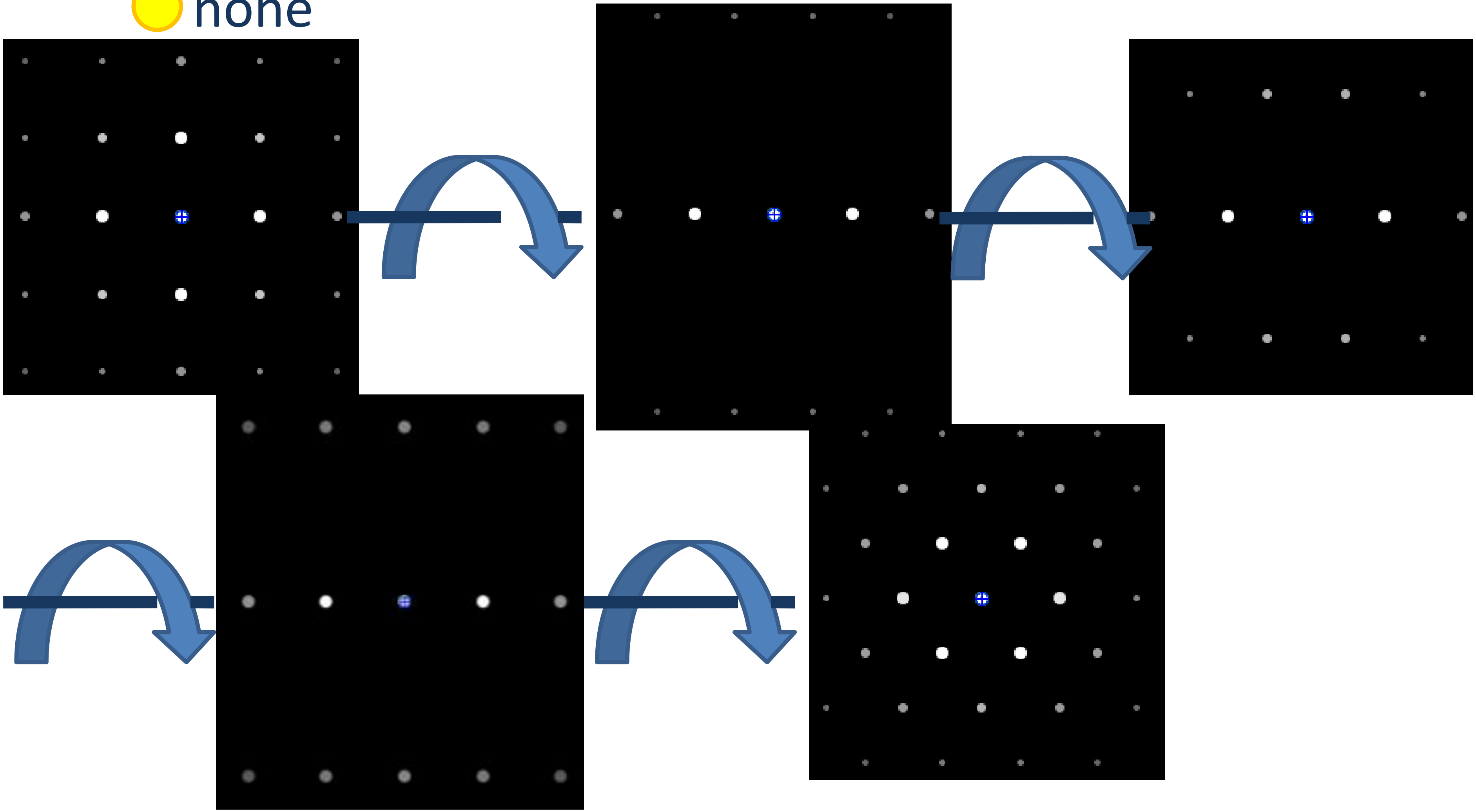


In SAED patterns there is always an inversion centre due to the diffraction geometry!



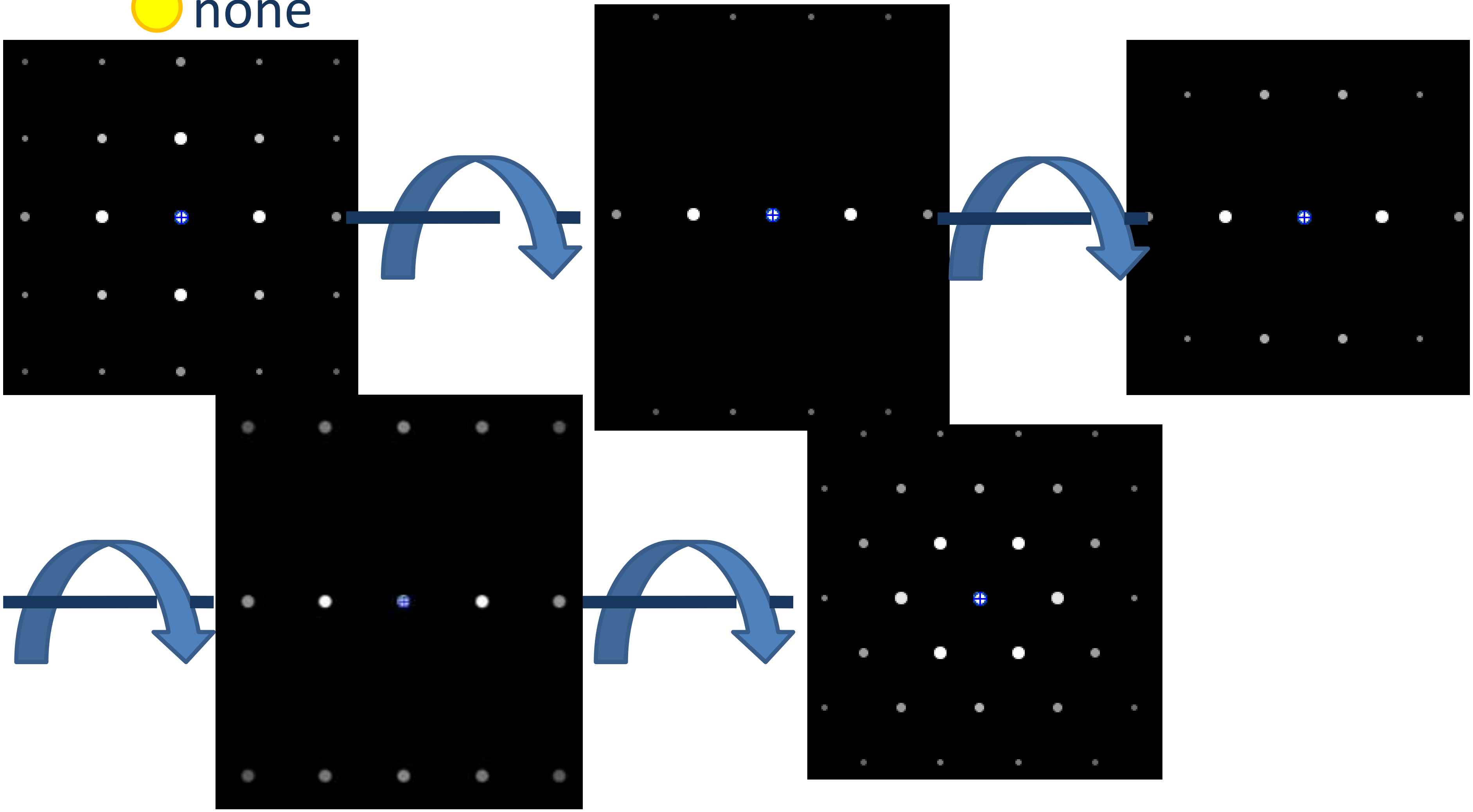
What crystal class has both 4-fold and 3-fold axes?

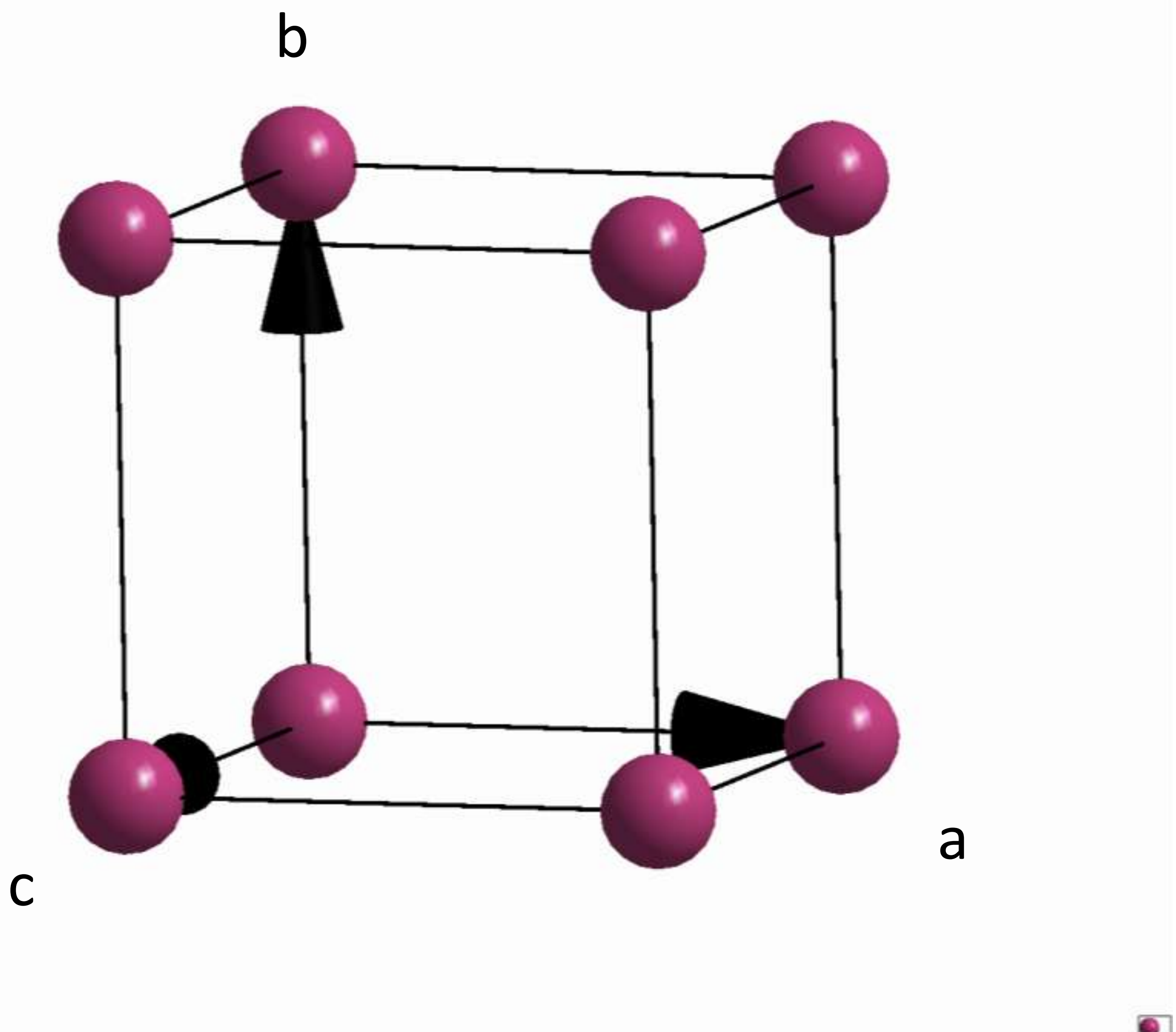
- cubic
- hexagonal
- none



What crystal class has both 4-fold and 3-fold axes?

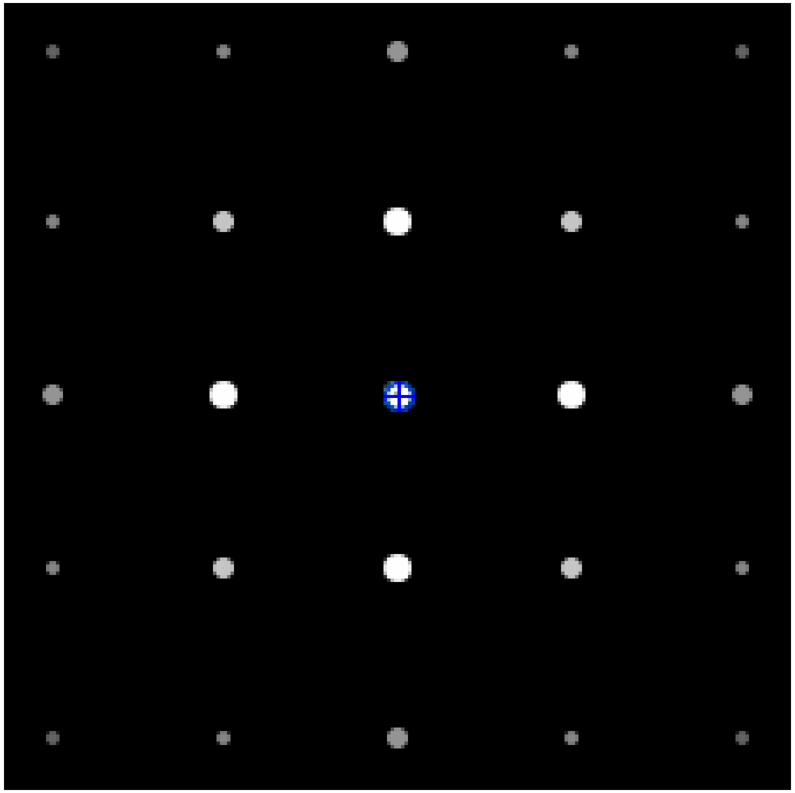
- cubic
- hexagonal
- none




b
a
c

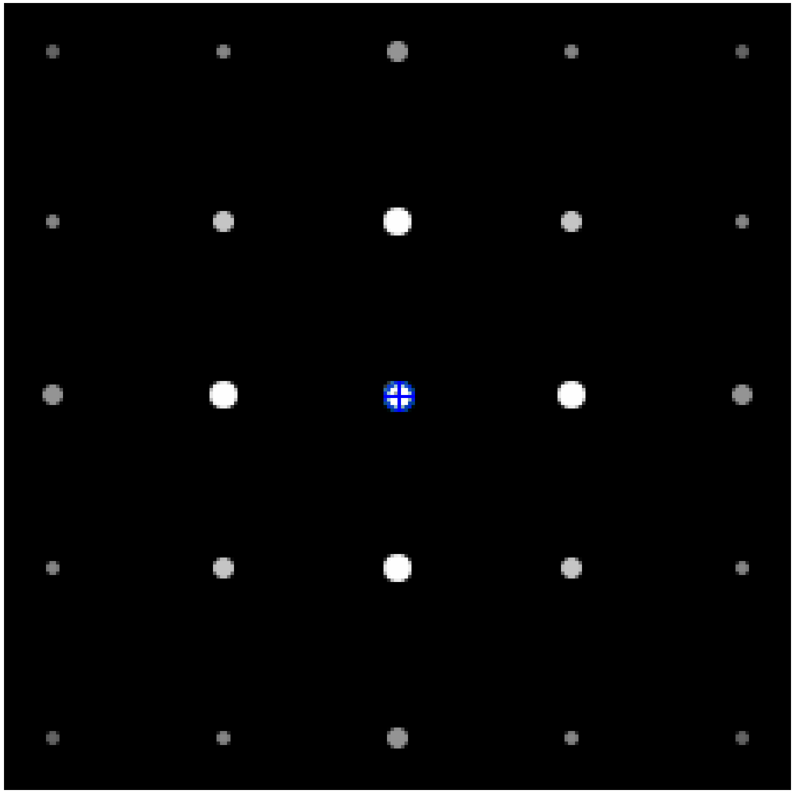
How many possible choices for the basic vectors are there on this square pattern?

- 1
- 2
- more



How many possible choices for the basic vectors are there on this square pattern?

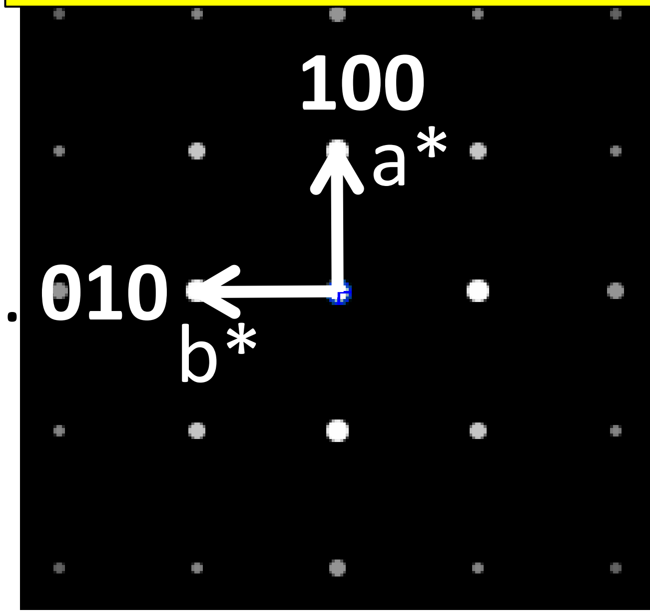
- 1
- 2
- more

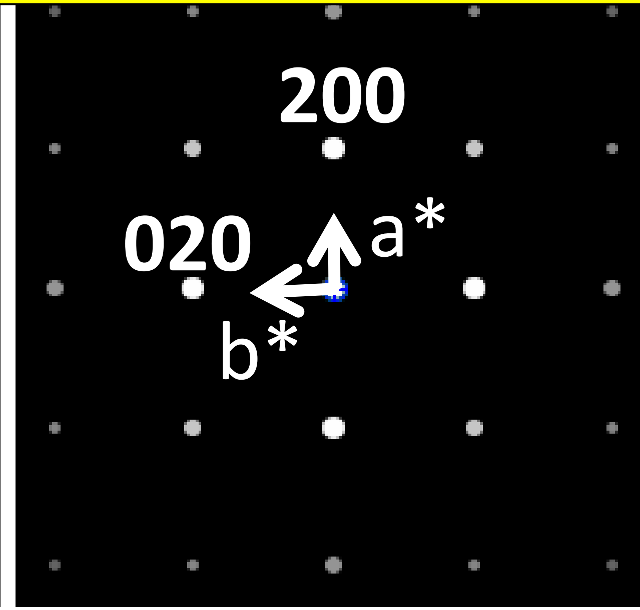


There can be a reflection condition!

hk0:

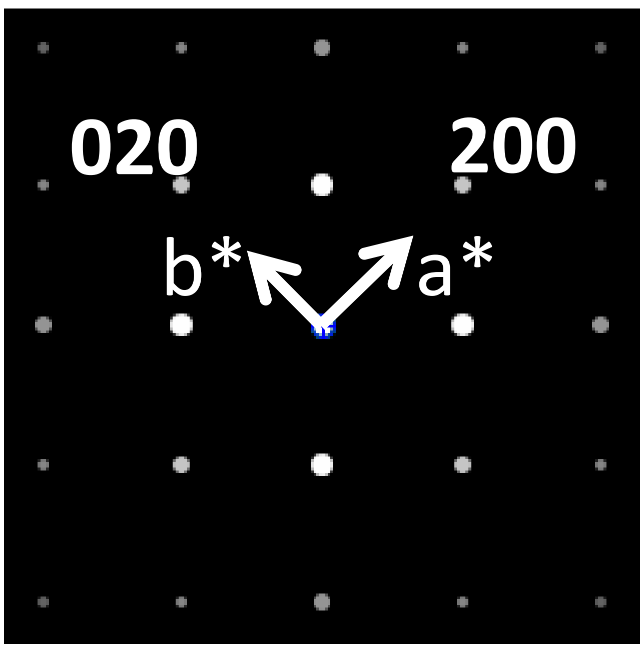
no cond.





h=2n,
k=2n

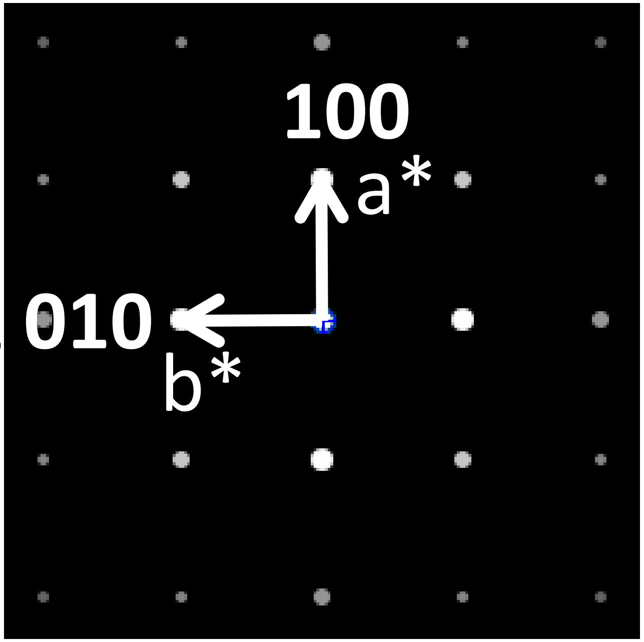
h+k=2n



Choose simplest first and see if ok with other zones.

hk0:

no cond.



Measure R

Calculate d from R.d=λL (known)

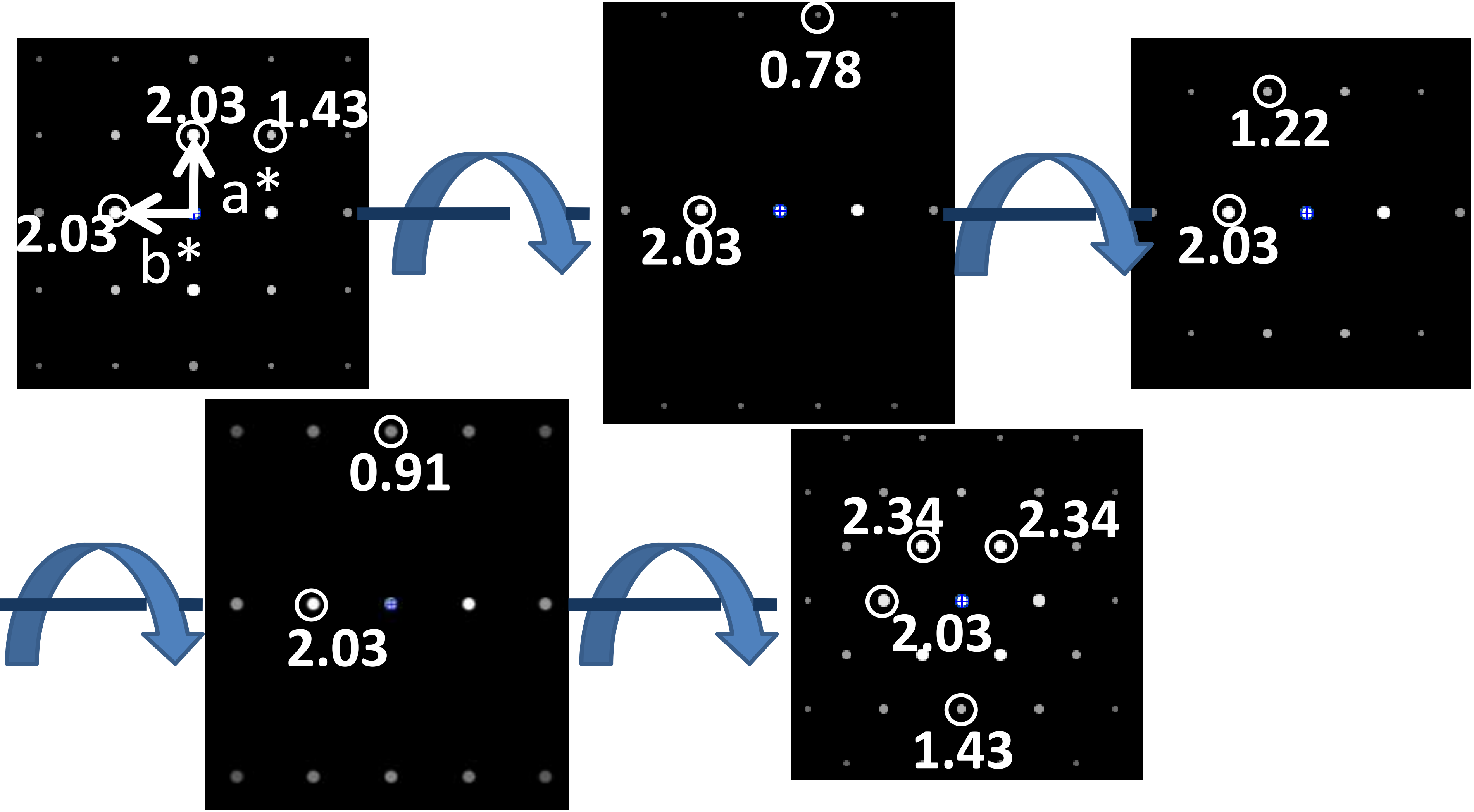
Determine a, b, c

Make list of d-spacings

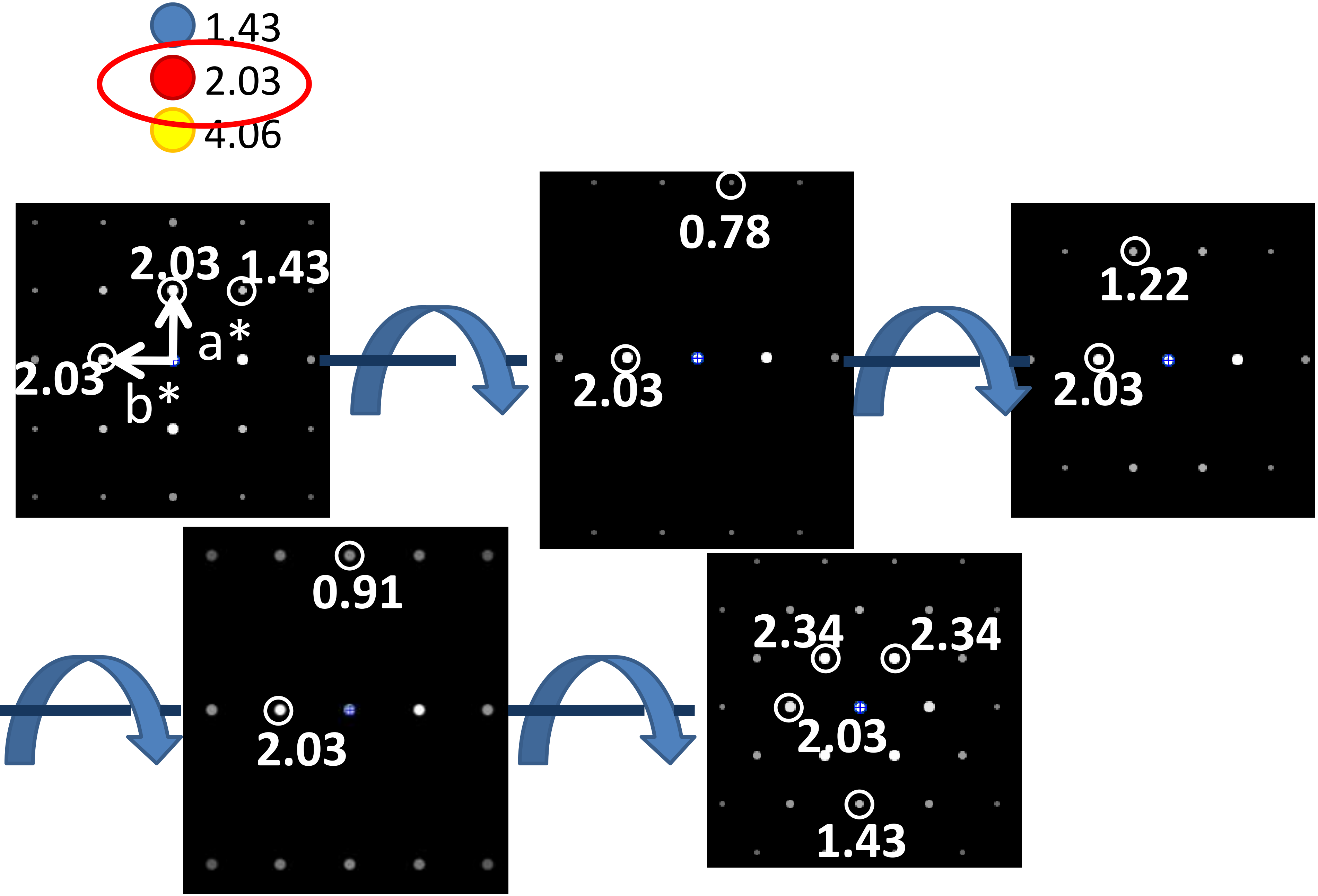
Check if you can index the other patterns with this

What will be the value of a and b with this choice?

- 1.43
- 2.03
- 4.06



What will be the value of a and b with this choice?



If no reflection condition:
a=b= c=2.03 Å

list of d-spacings freeware: Powdercell

H	K	L	d/Å
1	0	0	2.03000
1	1	0	1.43543
1	1	1	1.17202
2	0	0	1.01500
2	1	0	0.90784
2	1	1	0.82874

Can you index all observed reflections using these cell parameters?

- yes
- no

If no reflection condition:

a=b= c=2.03 Å

list of d-spacings freeware: Powdercell

H	K	L	d/Å
1	0	0	2.03000
1	1	0	1.43543
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Can you index all observed reflections using these cell parameters?

- yes
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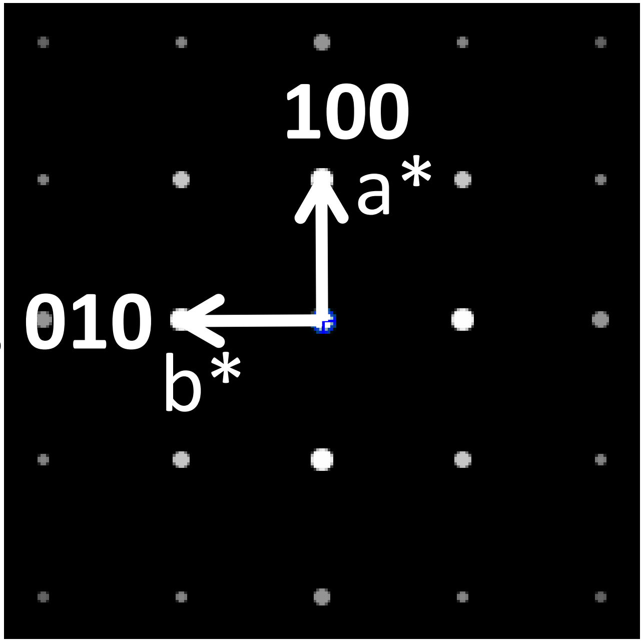
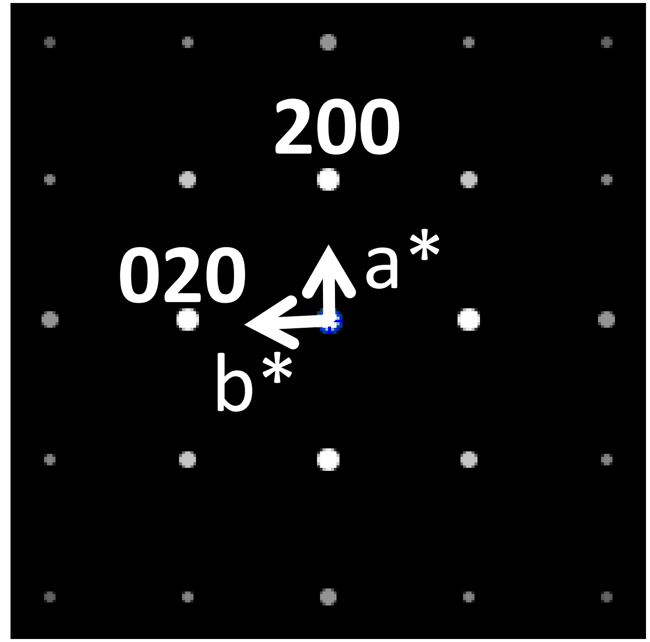
hk0:

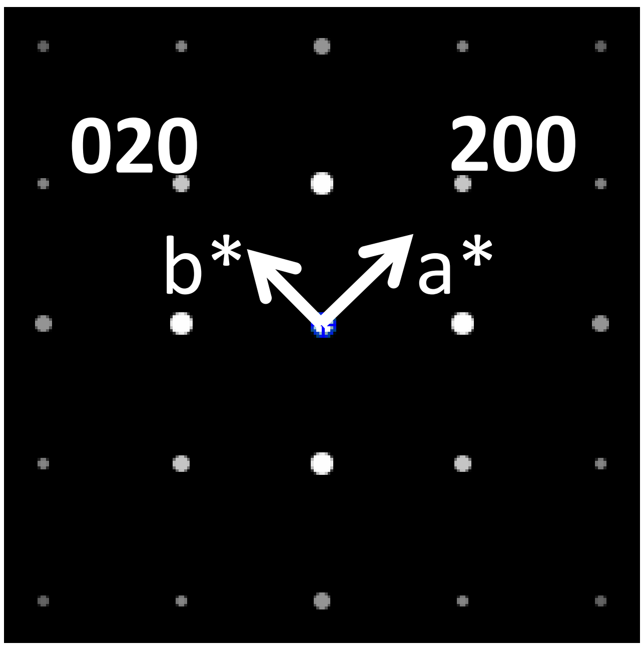
no cond.





h=2n,
k=2n

h+k=2n



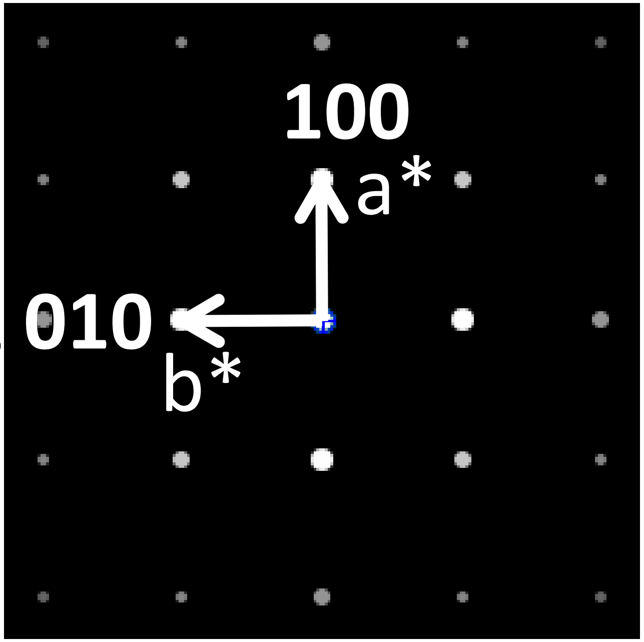
Increase the cell parameters to the next possibility...

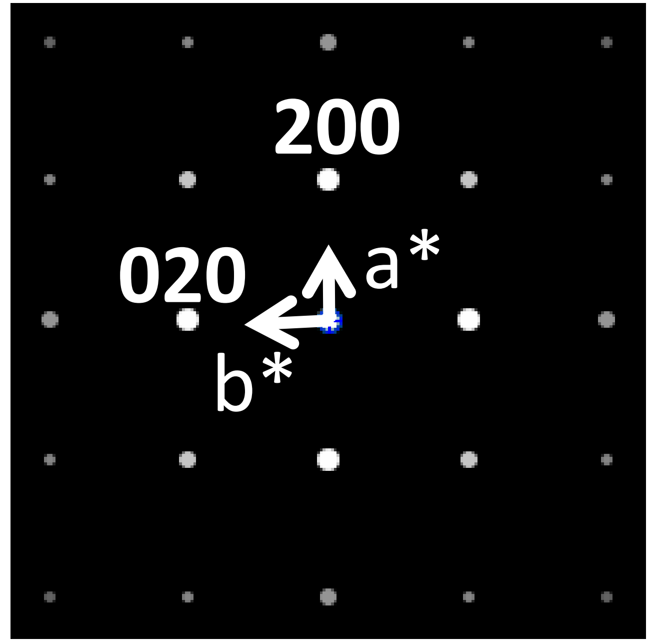
Which one has second smallest cell parameters?

- top
- left

hk0:

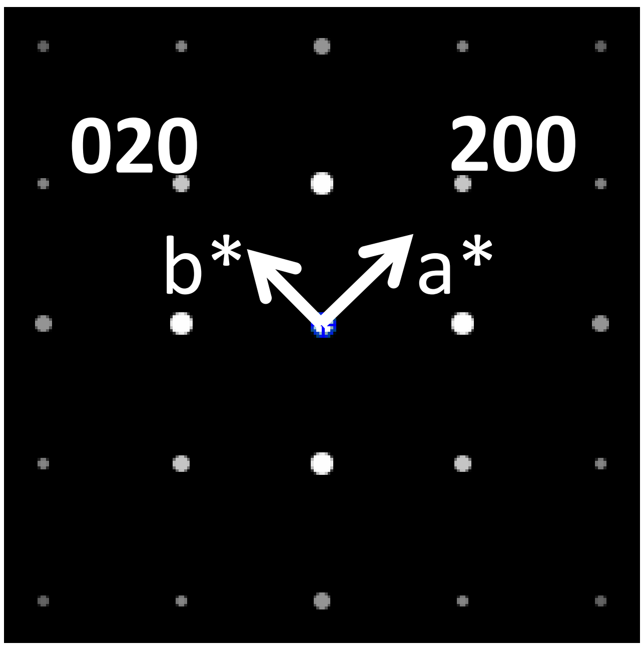
no cond.





h=2n,
k=2n

h+k=2n



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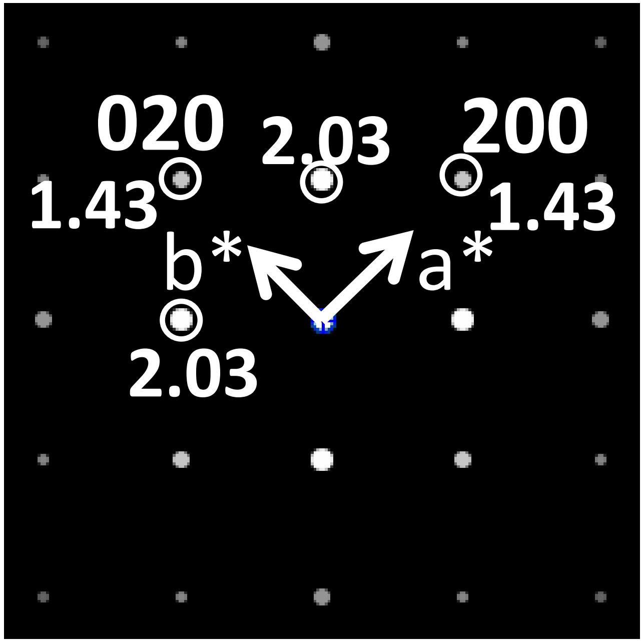
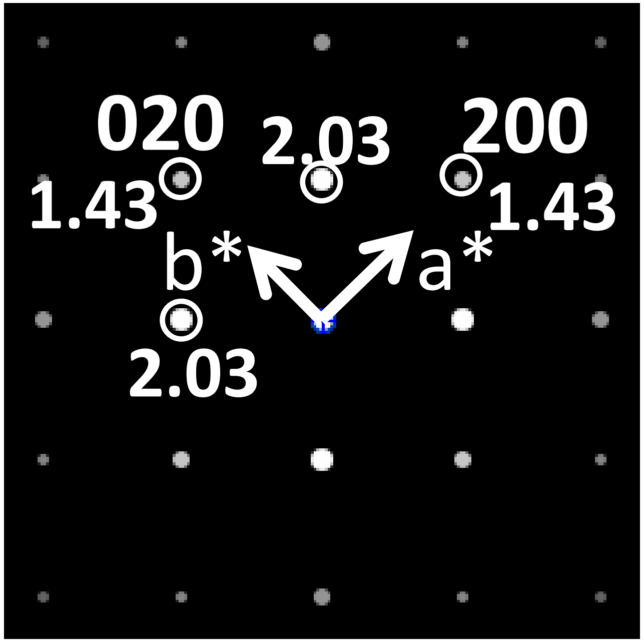


In this case, a=b=

- 1.43 Å
- 2.03 Å
- 2.86 Å

h+k=2n



In this case, a=b=

- 1.43 Å
- 2.03 Å
- 2.86 Å

If hk0:h+k=2n, then a=b= 2.86 Å

list of d-spacings, Powdercell:

H	K	L	d/Å
1	0	0	2,86000
1	1	0	2,02233
1	1	1	1,65122
2	0	0	1,43000
2	1	0	1,27903
2	1	1	1,16759
2	2	0	1,01116
3	0	0	0,95333
2	2	1	0,95333
3	1	0	0,90441
3	1	1	0,86232
2	2	2	0,82561
3	2	0	0,79322

Can you index all observed reflections using these cell parameters?

- yes
- no

If hk0:h+k=2n, then a=b= 2.86 Å

list of d-spacings, Powdercell:

H	K	L	d/Å
1	0	0	2,86000
1	1	0	2,02233
1	1	1	1,65122
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3	1	0	0,90441
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2	2	2	0,82561
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2	2	0	1,01116
3	0	0	0,95333
2	2	1	0,95333
3	1	0	0,90441
3	1	1	0,86232
2	2	2	0,82561
3	2	0	0,79322

I show also the reflections not in agreement with hk0: h+k=2n.
Will they be seen on any of the SAED patterns of the tilt series?

- it is possible
- always
- never

If hk0:h+k=2n, then a=b= 2.86 Å

list of d-spacings, Powdercell:

H	K	L	d/Å
1	0	0	2,86000
1	1	0	2,02233
1	1	1	1,65122
2	0	0	1,43000
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2	1	1	1,16759
2	2	0	1,01116
3	0	0	0,95333
2	2	1	0,95333
3	1	0	0,90441
3	1	1	0,86232
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3	2	0	0,79322

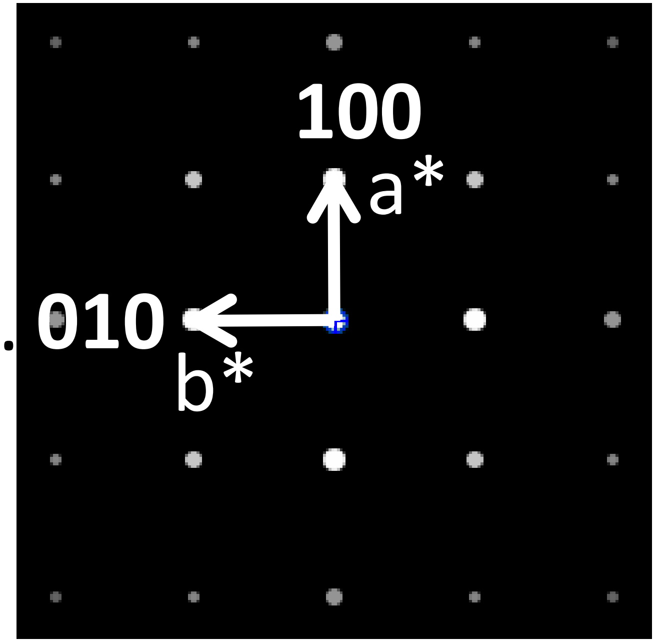
I show also the reflections not in agreement with hk0: h+k=2n.

Will they be seen on any of the SAED patterns of the tilt series?

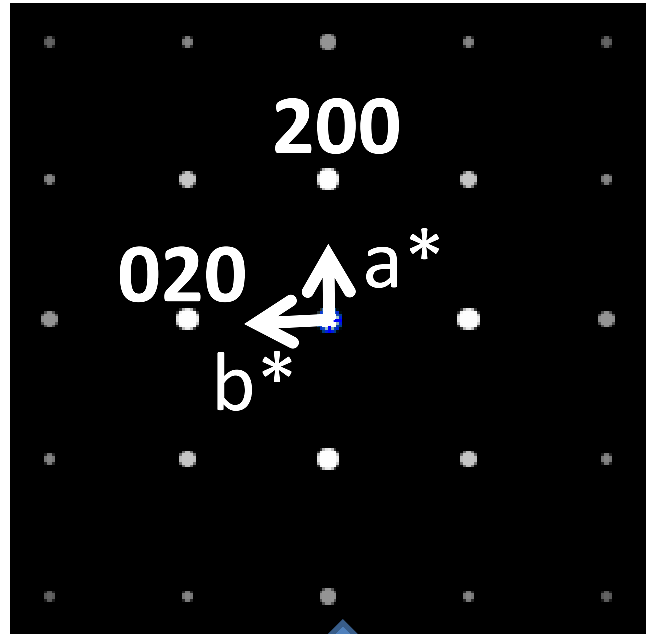
- it is possible
- always
- never

hk0:

no cond.

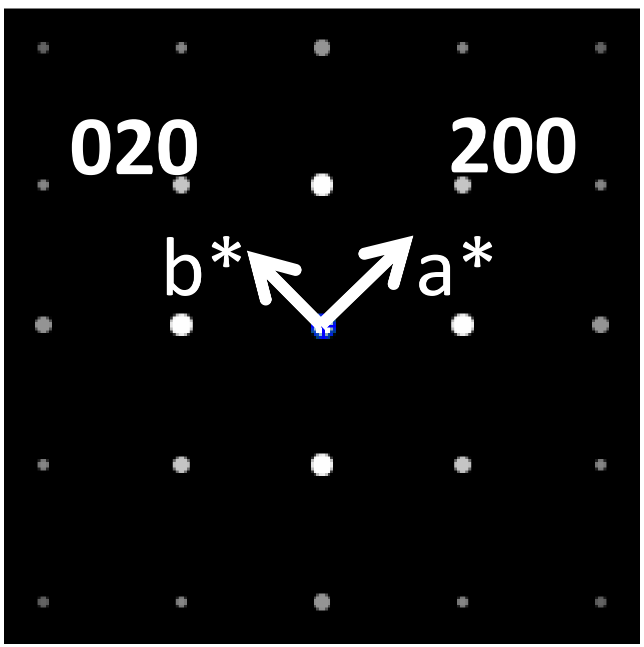


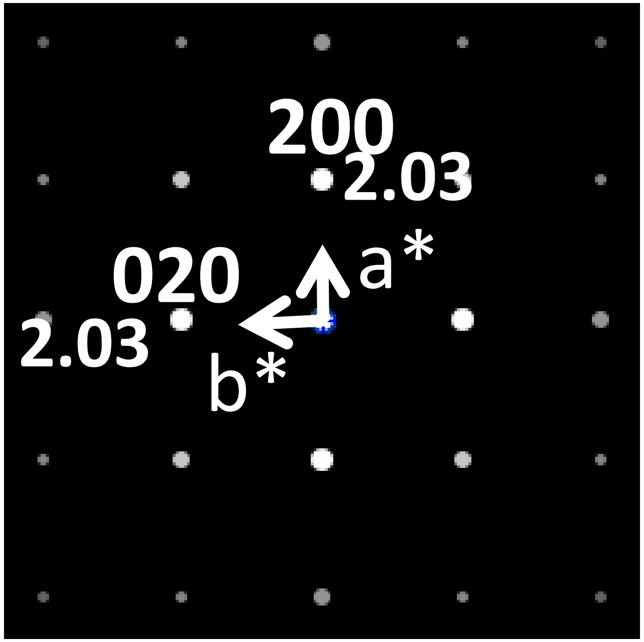
h=2n,
k=2n



Next possibility...

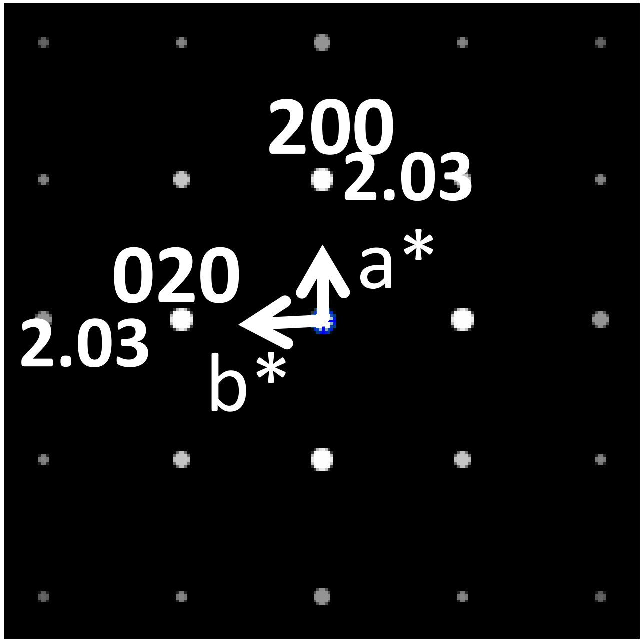
h+k=2n





In this case, a=b=

- 2.03 Å
- 4.06 Å
- 5.92 Å



In this case, a=b=

- 2.03 Å
- 4.06 Å
- 5.92 Å

If hk0:h,k=2n, then a=b= 4.06 Å

list of d-spacings, Powdercell:

H	K	L	d/Å
1	0	0	4,06000
1	1	0	2,87085
1	1	1	2,34404
2	0	0	2,03000
2	1	0	1,81569
2	1	1	1,65749
2	2	0	1,43543
3	0	0	1,35333
2	2	1	1,35333
3	1	0	1,28388
3	1	1	1,22414
2	2	2	1,17202
3	2	0	1,12604
3	2	1	1,08508
4	0	0	1,01500
4	1	0	0,98469
3	2	2	0,98469
4	1	1	0,95695
3	3	0	0,95695
3	3	1	0,93143
4	2	0	0,90784
4	2	1	0,88596
3	3	2	0,86559
4	2	2	0,82874
5	0	0	0,81200
4	3	0	0,81200
5	1	0	0,79623
4	3	1	0,79623
5	1	1	0,78135
3	3	3	0,78135

Can you index all observed reflections with these cell parameters?

- yes
- no

Do it now.

If hk0:h,k=2n, then a=b= 4.06 Å

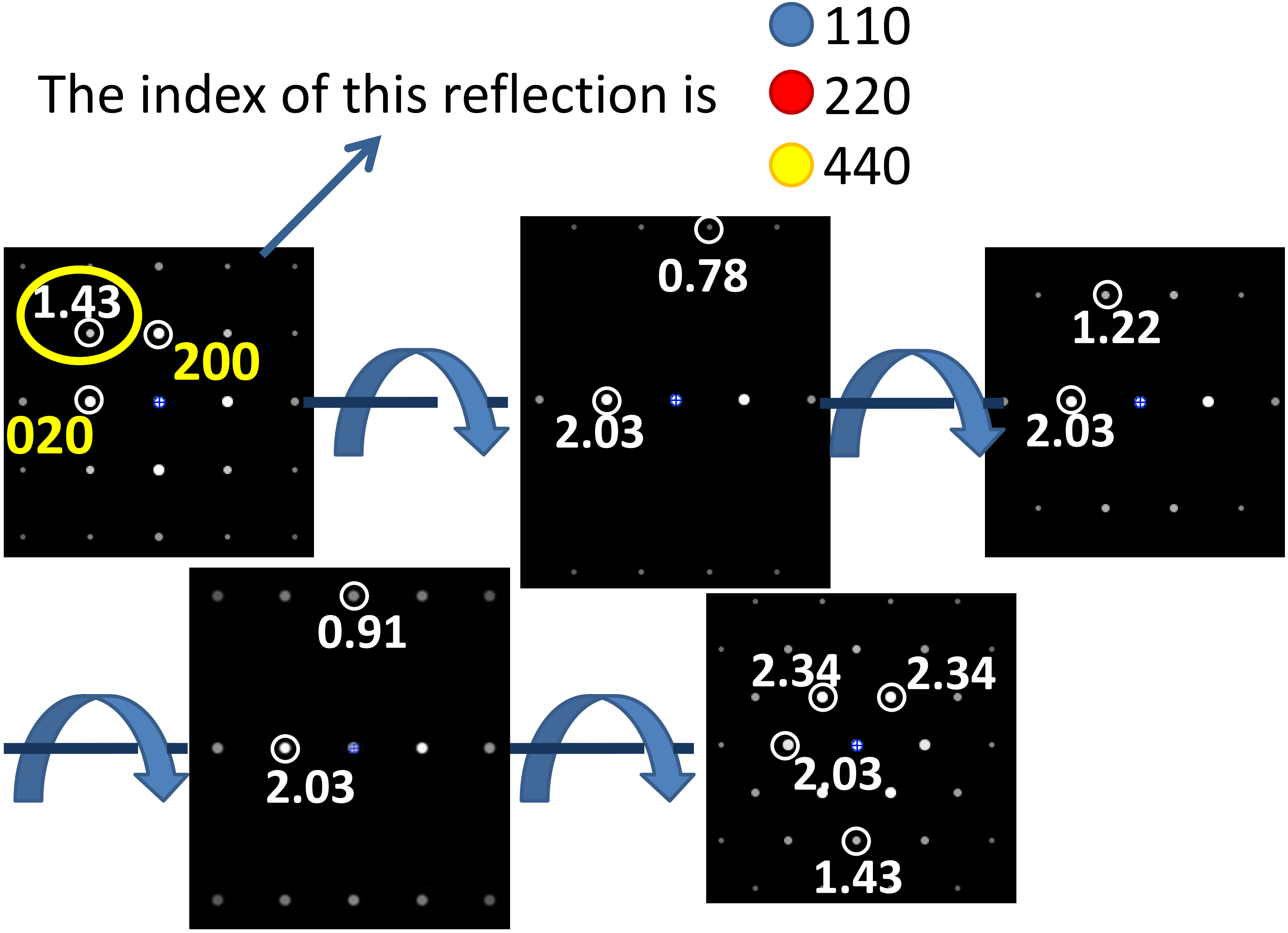
list of d-spacings, Powdercell:

H	K	L	d/Å
1	0	0	4,06000
1	1	0	2,87085
1	1	1	2,34404
2	0	0	2,03000
2	1	0	1,81569
2	1	1	1,65749
2	2	0	1,43543
3	0	0	1,35333
2	2	1	1,35333
3	1	0	1,28388
3	1	1	1,22414
2	2	2	1,17202
3	2	0	1,12604
3	2	1	1,08508
4	0	0	1,01500
4	1	0	0,98469
3	2	2	0,98469
4	1	1	0,95695
3	3	0	0,95695
3	3	1	0,93143
4	2	0	0,90784
4	2	1	0,88596
3	3	2	0,86559
4	2	2	0,82874
5	0	0	0,81200
4	3	0	0,81200
5	1	0	0,79623
4	3	1	0,79623
5	1	1	0,78135
3	3	3	0,78135

Can you index all observed reflections with these cell parameters?

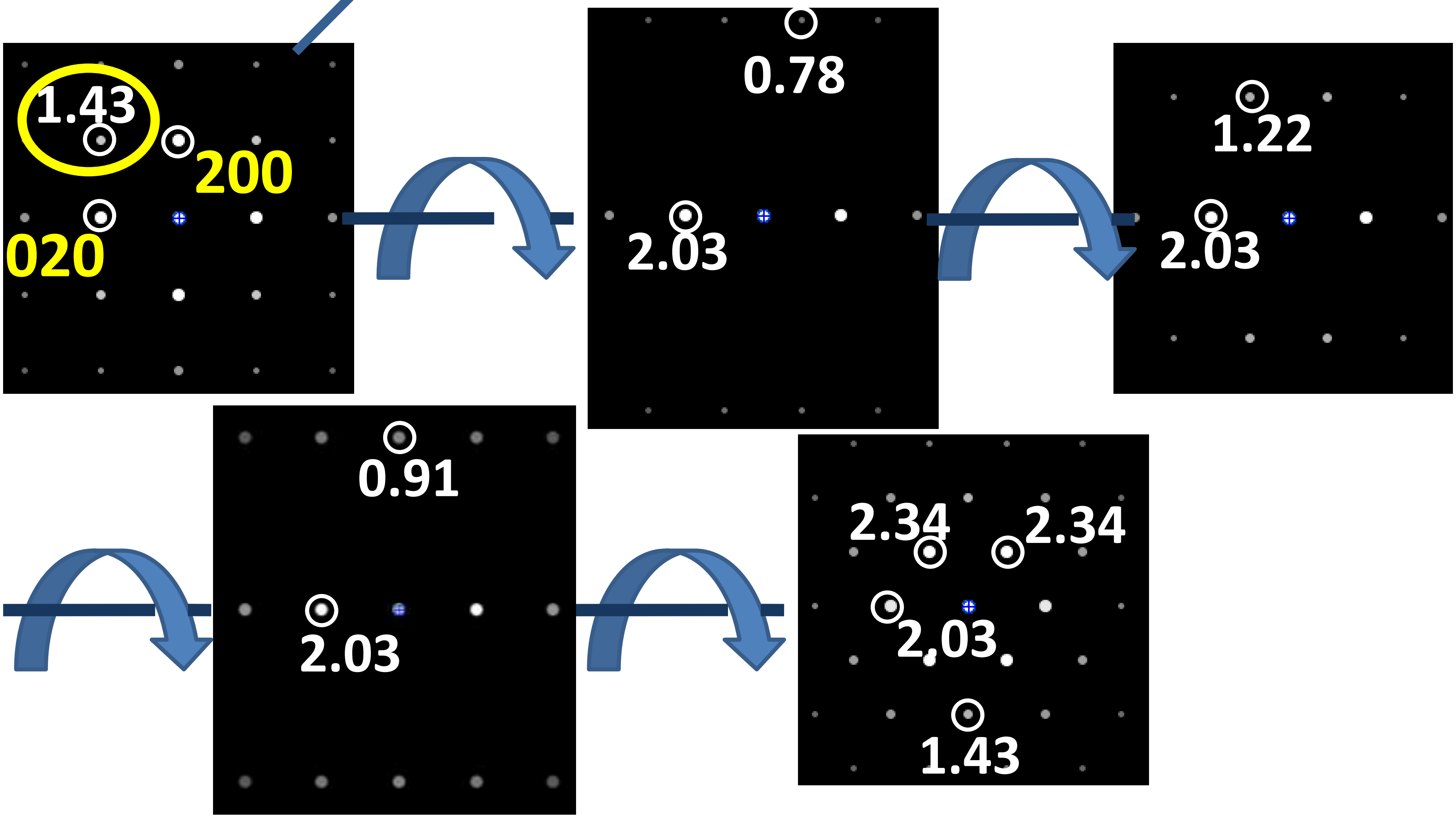
- yes
- no

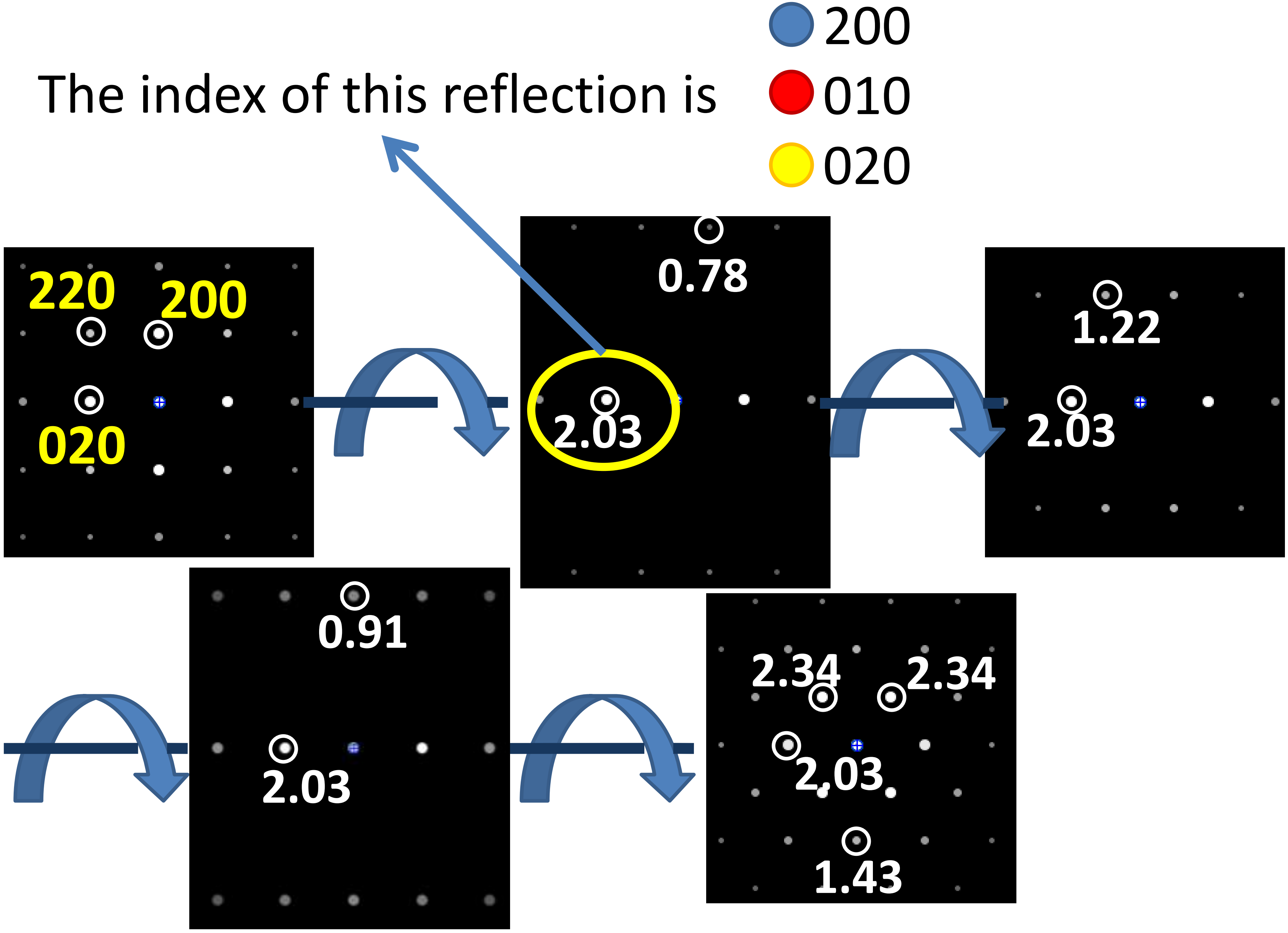
Do it now.


The index of this reflection is
110
220
440
1.43
200
020
0.78
2.03
1.22
2.03
0.91
2.03
2.34
2.34
2.03
1.43

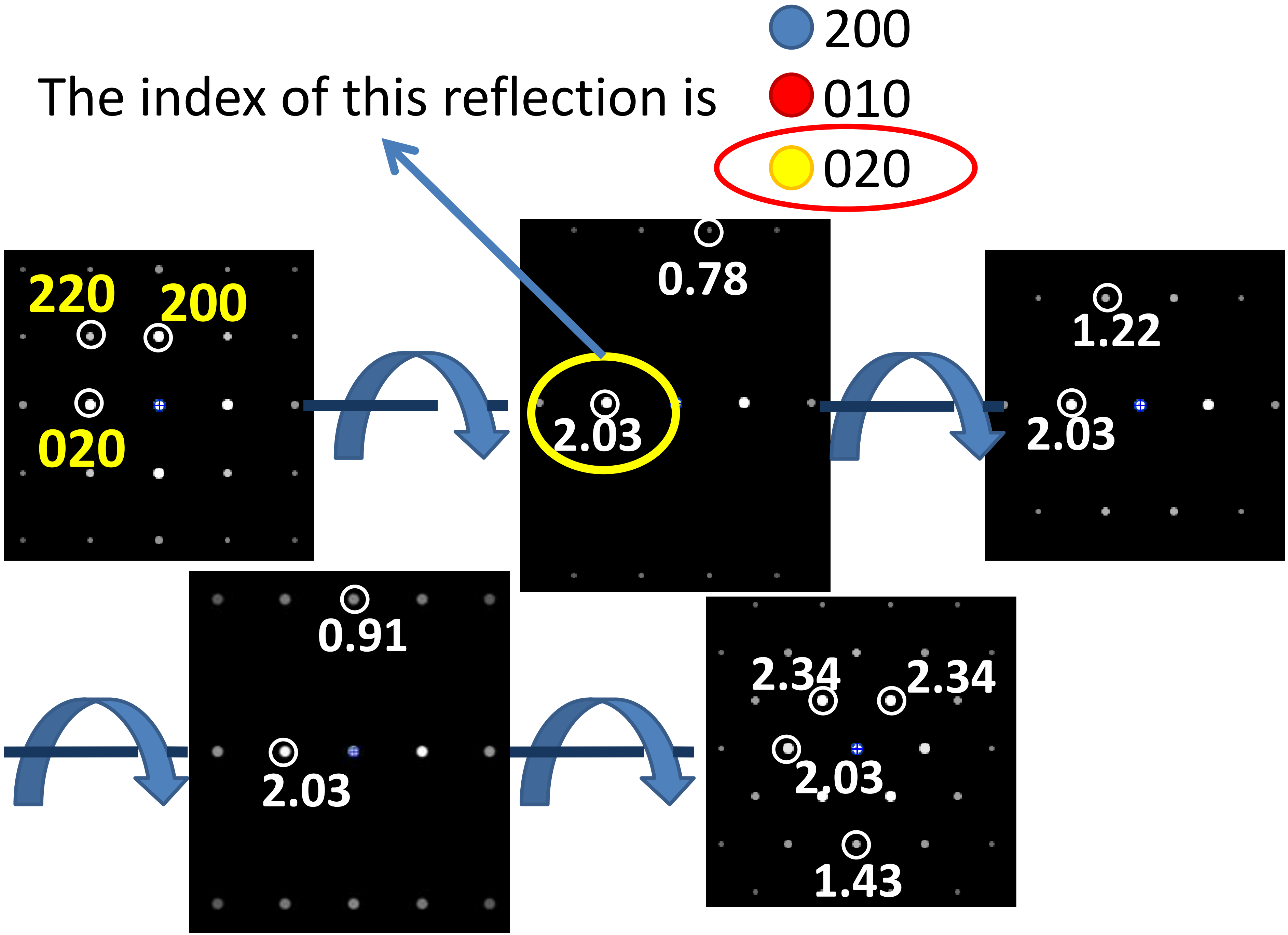
The index of this reflection is

- 110
- 220
- 440





The index of this reflection is
200
010
020
220
200
020
0.78
2.03
1.22
2.03
0.91
2.03
2.34
2.34
2.03
1.43

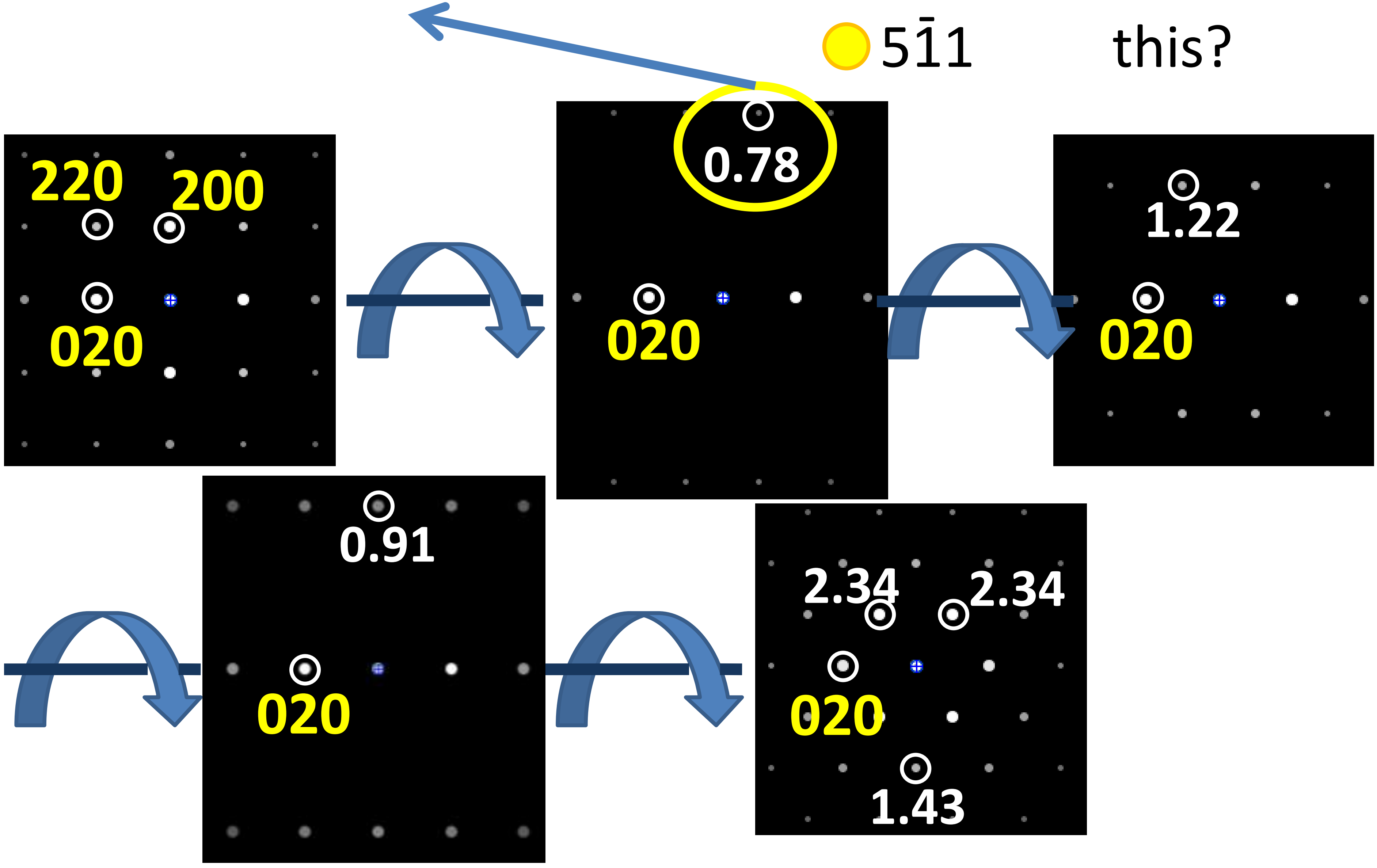


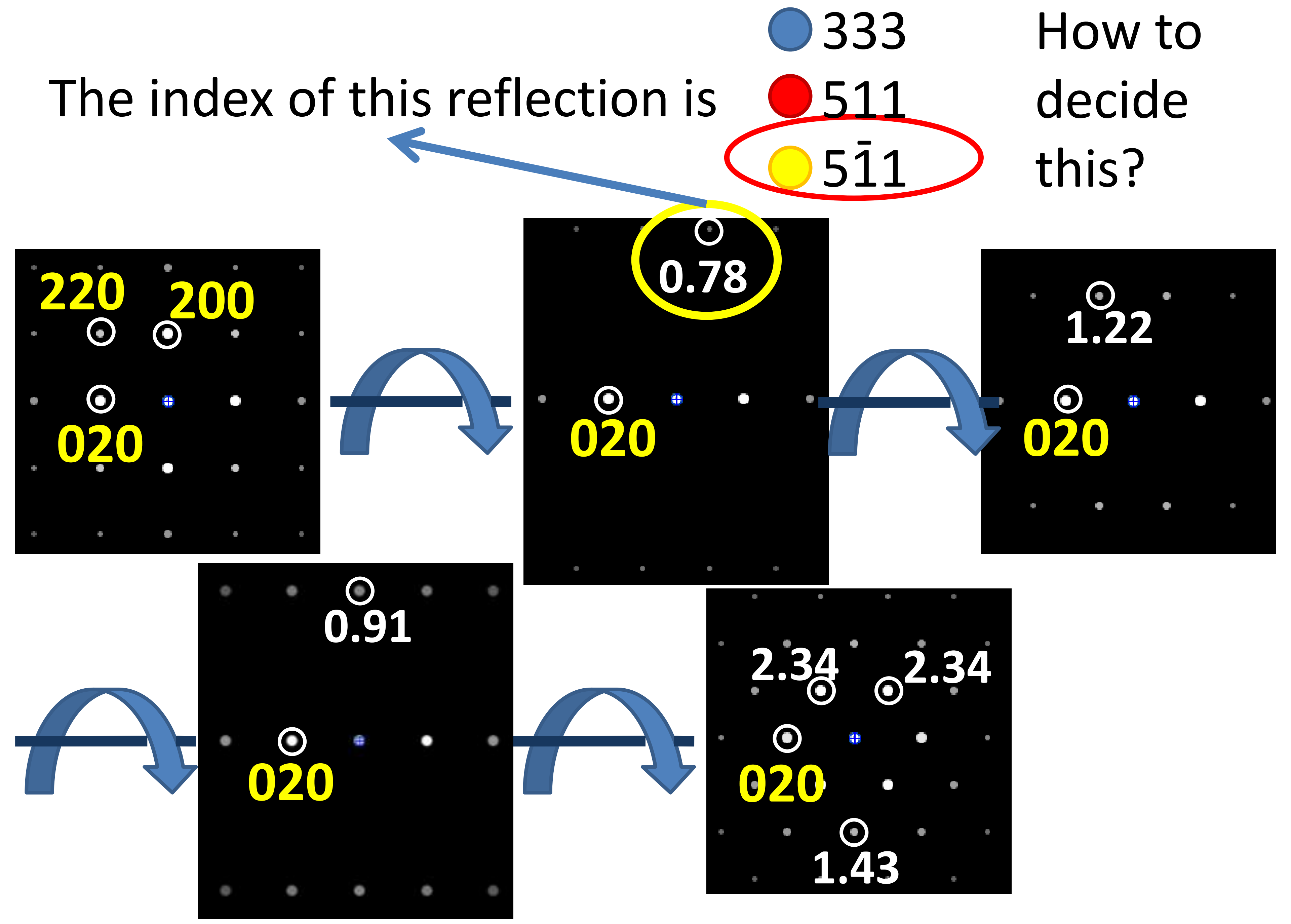
The index of this reflection is
200
010
020
220
200
020
0.78
2.03
1.22
2.03
0.91
2.03
2.34
2.34
2.03
1.43

The index of this reflection is

- 333
- 511
- $5\bar{1}1$

How to decide this?





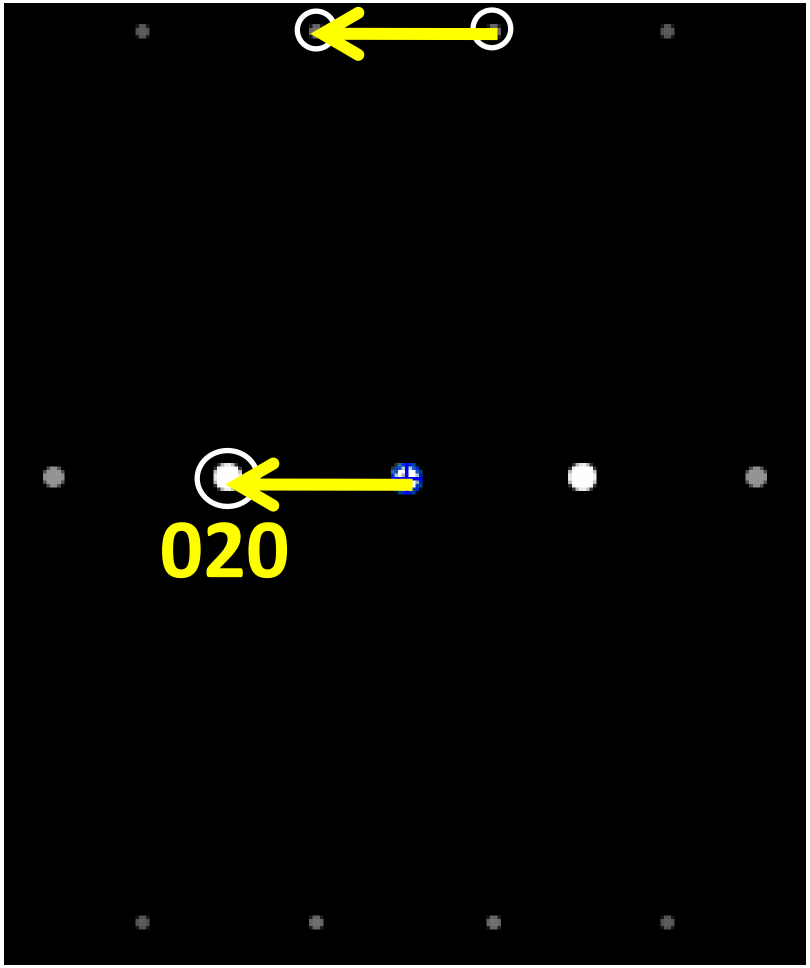
The index of this reflection is
333
511
$5\bar{1}1$
How to decide this?
220
200
020
0.78
020
1.22
020
0.91
020
2.34
2.34
020
1.43

The index of this reflection is

~~333~~

511

$5\bar{1}1$



511 and $5\bar{1}1$?

115 and $1\bar{1}5$?

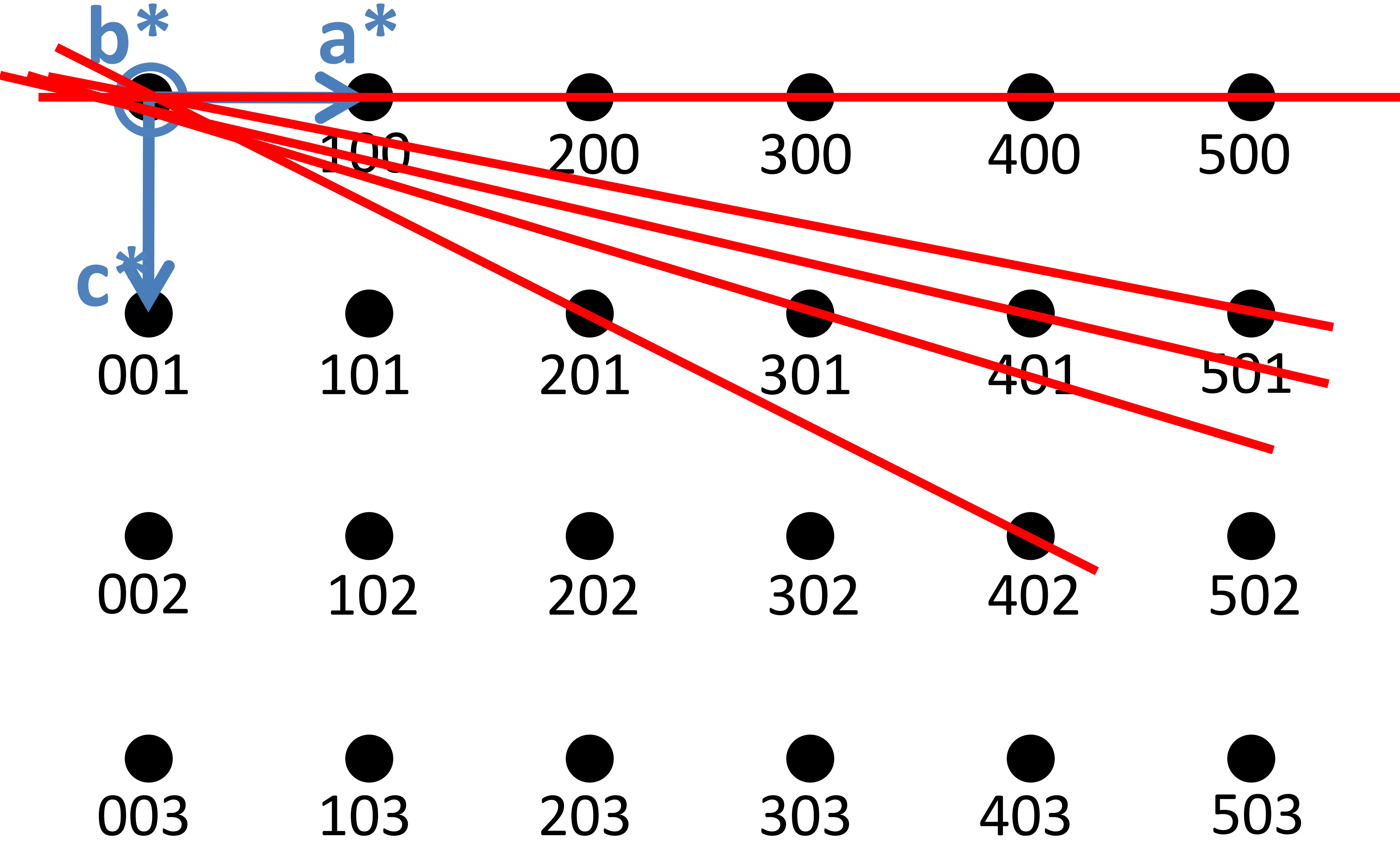
$51\bar{1}$ and $5\bar{1}\bar{1}$?

$\bar{1}15$ and $\bar{1}\bar{1}5$?

Calculate angles etc (lectures Mon-Wed)

or

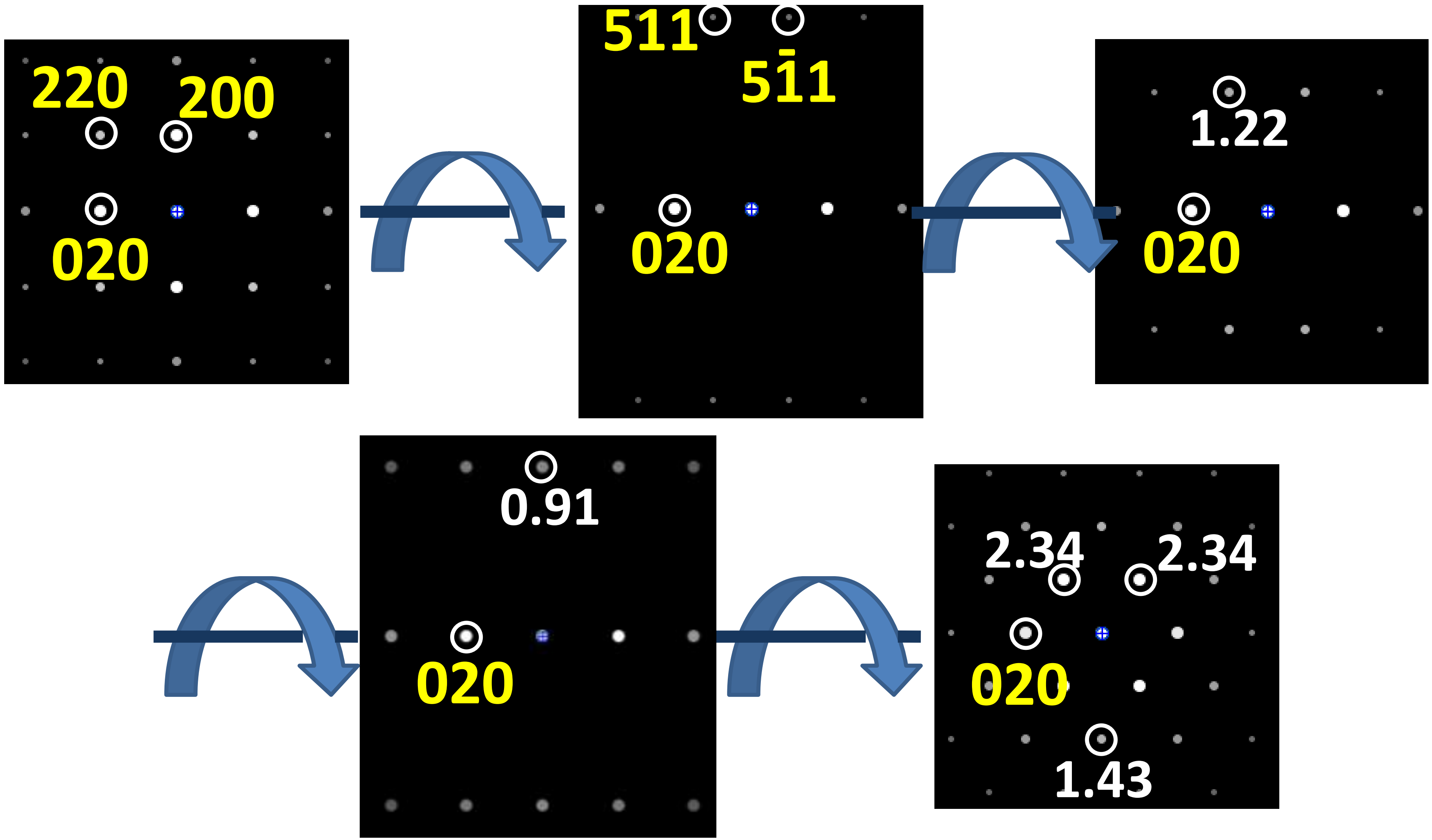
just do it graphically...



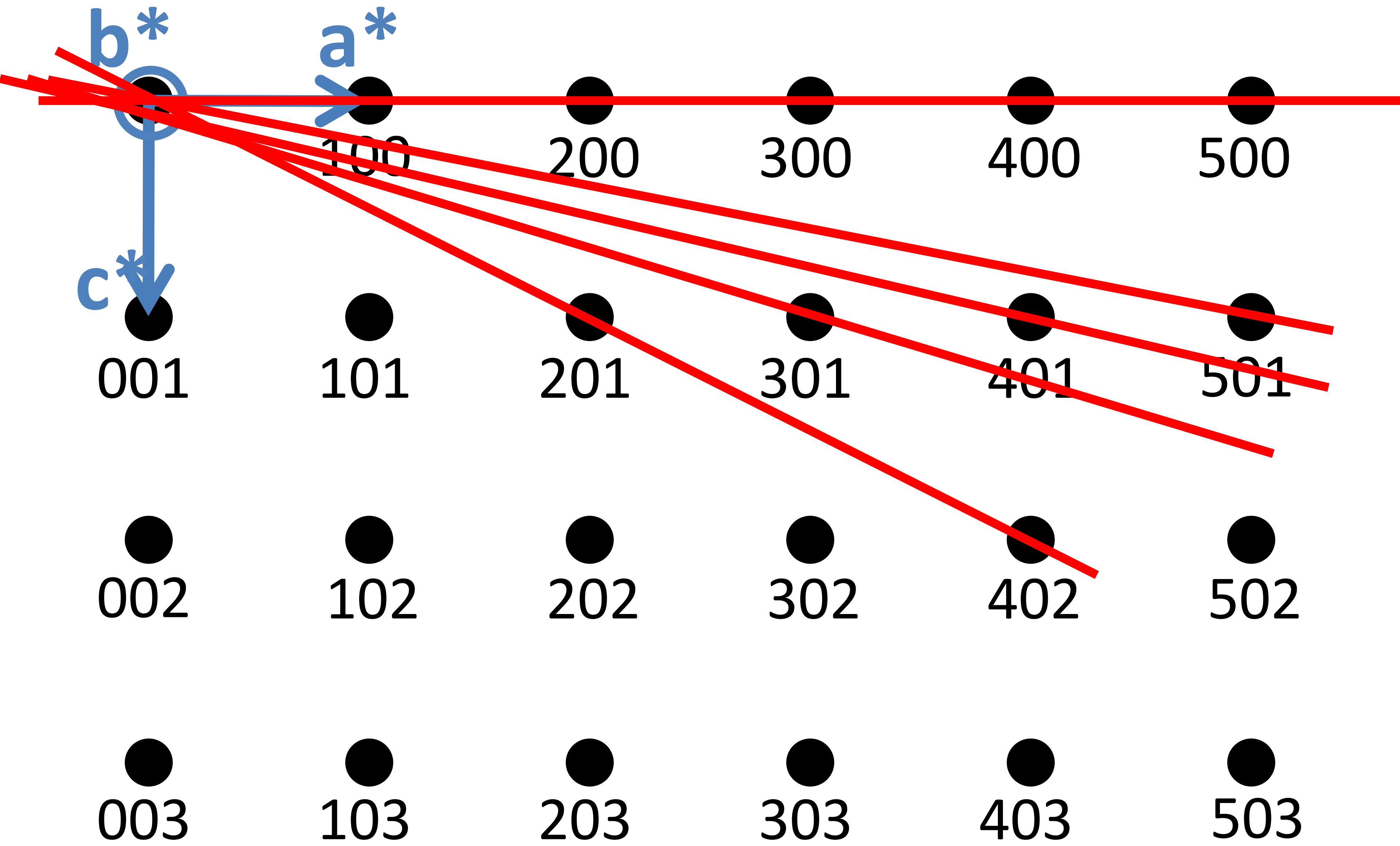
b*
a*
c*
100
200
300
400
500
001
101
201
301
401
501
002
102
202
302
402
502
003
103
203
303
403
503

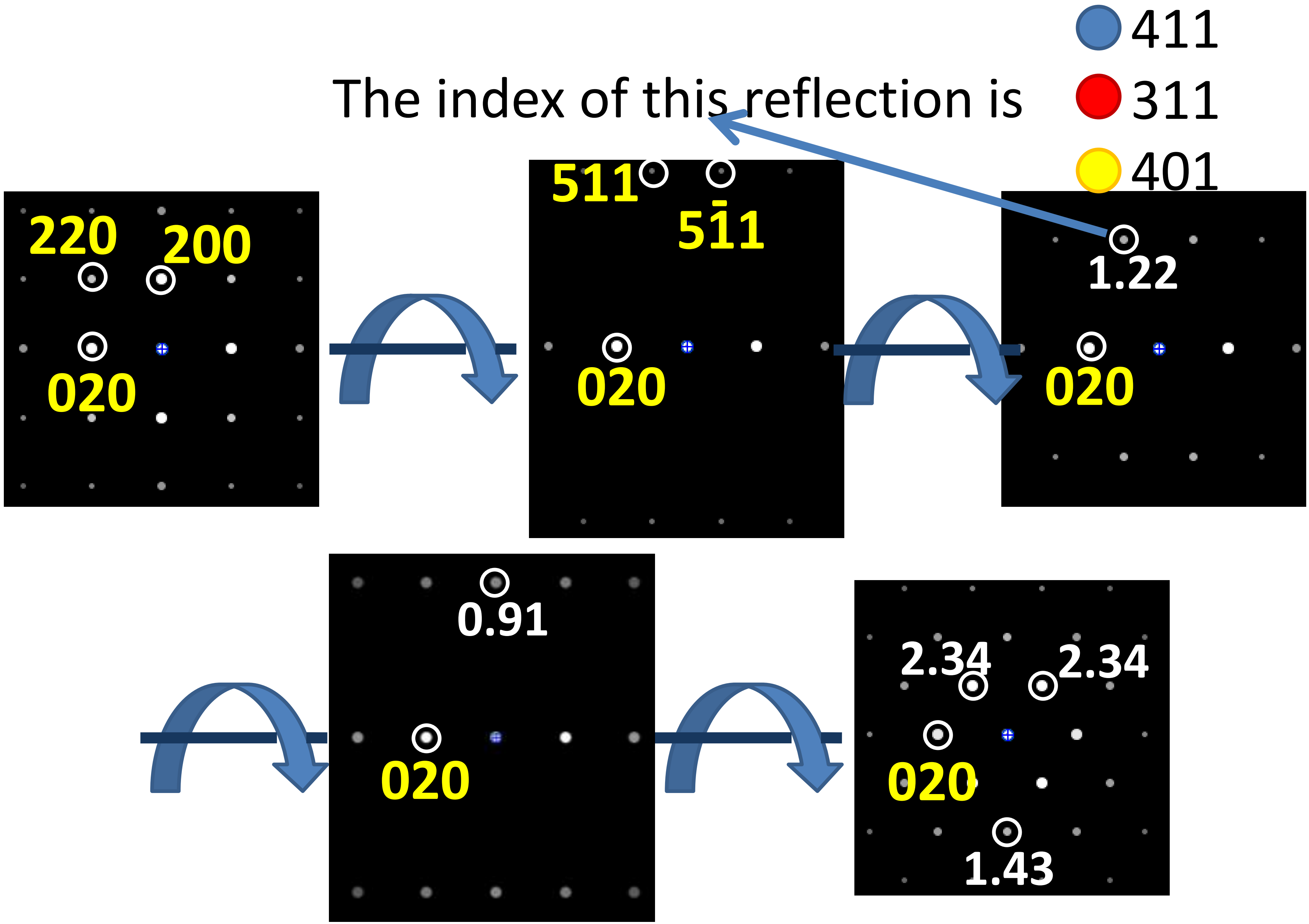
The index of this reflection is

- 333
- 511
- $5\bar{1}1$

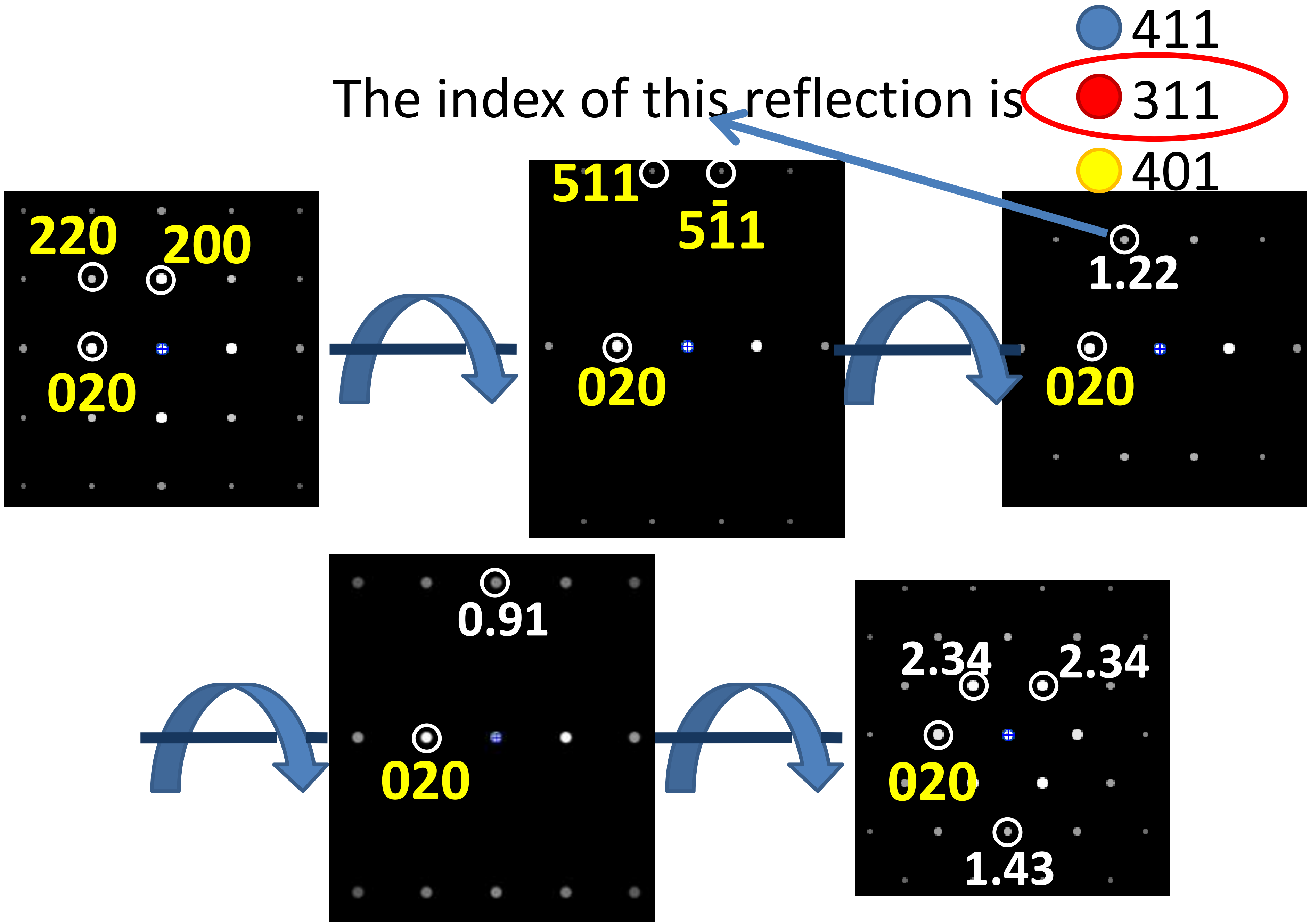


220
200
020
511
5$\bar{1}$1
020
1.22
020
0.91
020
2.34
2.34
020
1.43

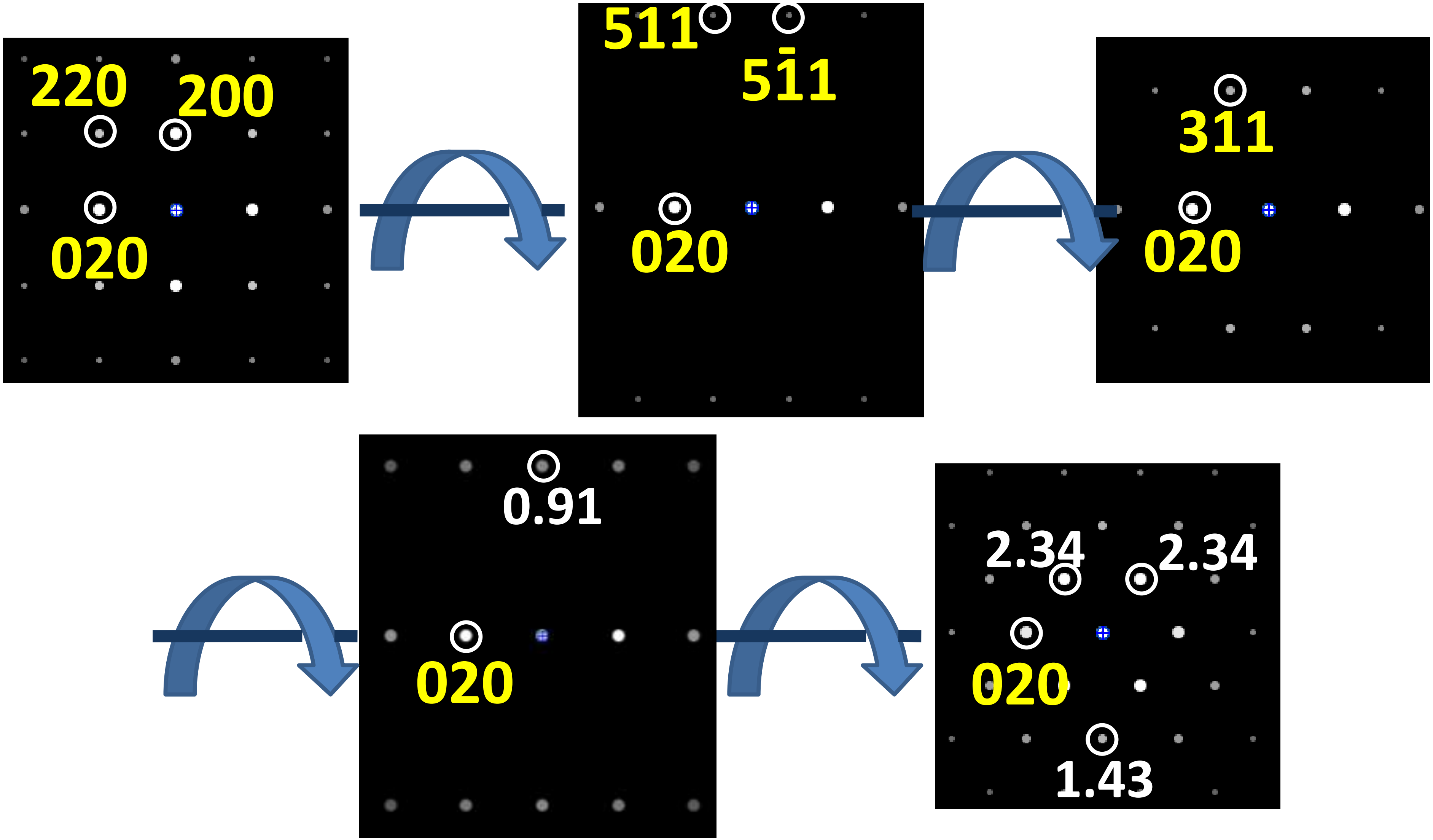

b*
a*
c*
100
200
300
400
500
001
101
201
301
401
501
002
102
202
302
402
502
003
103
203
303
403
503



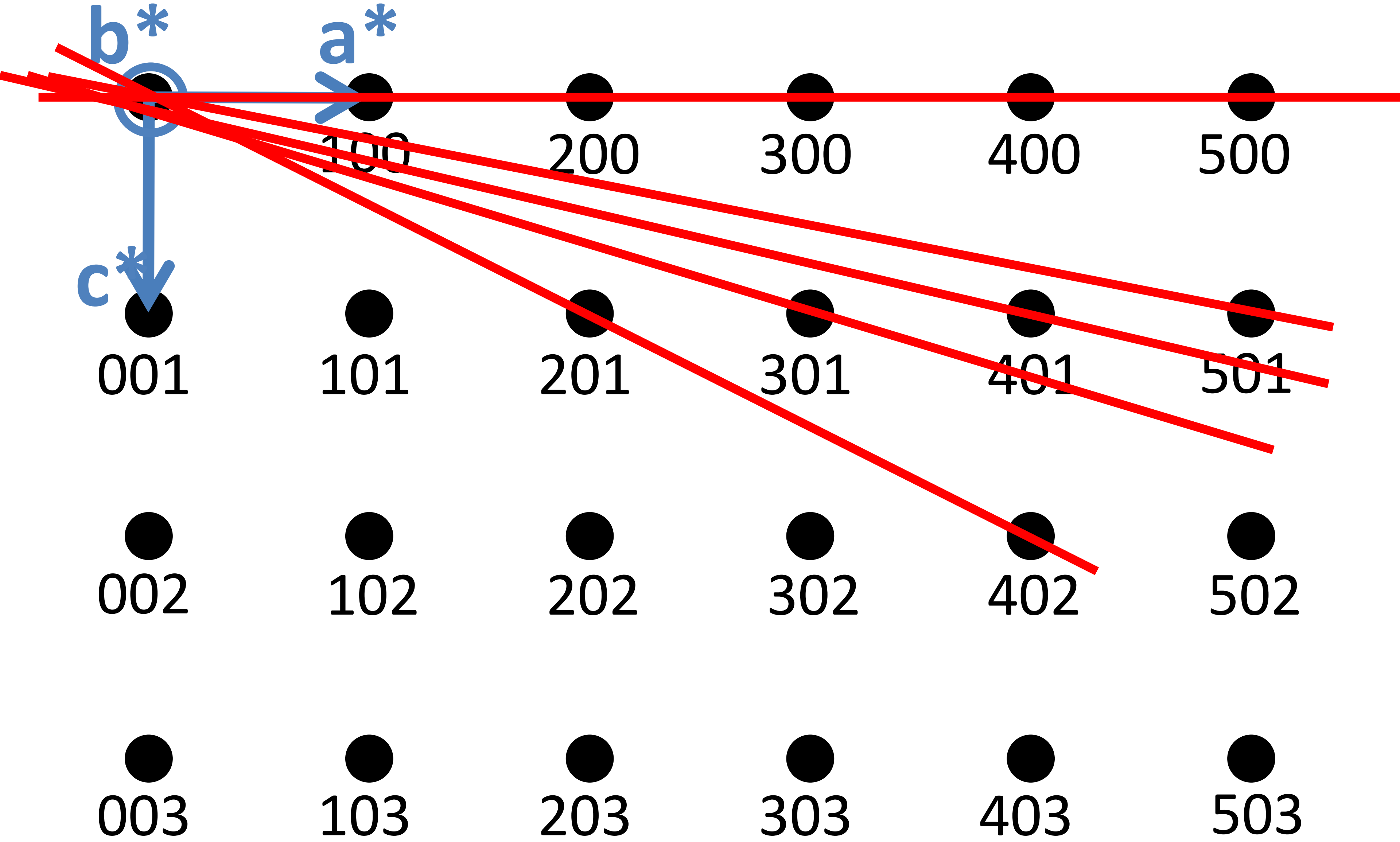
411
311
401
The index of this reflection is
220
200
020
511
5$\bar{1}$1
020
1.22
020
0.91
020
2.34
2.34
020
1.43



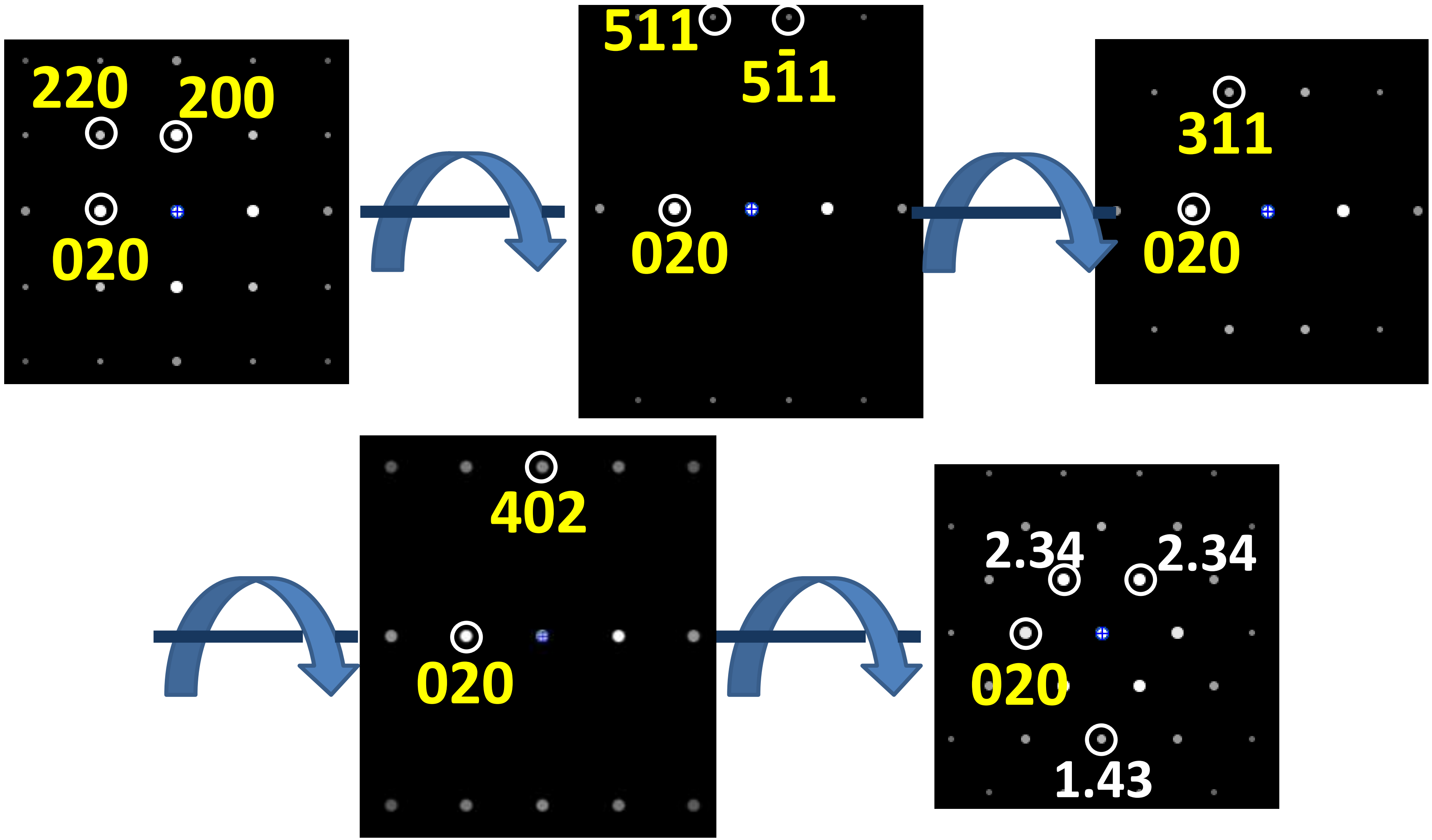
411
The index of this reflection is
311
401
220
200
020
511
5$\bar{1}$1
020
1.22
020
0.91
020
2.34
2.34
020
1.43

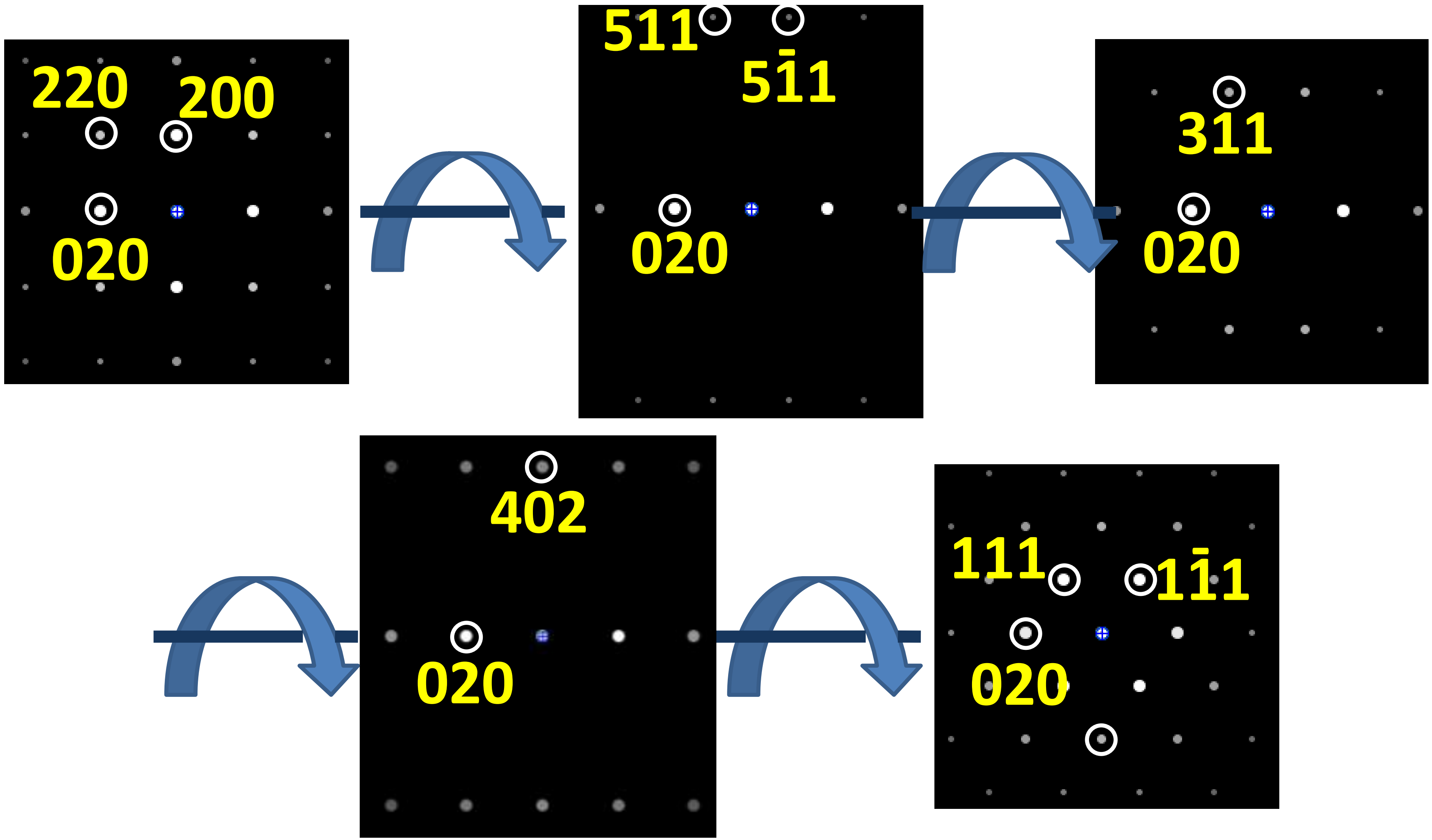


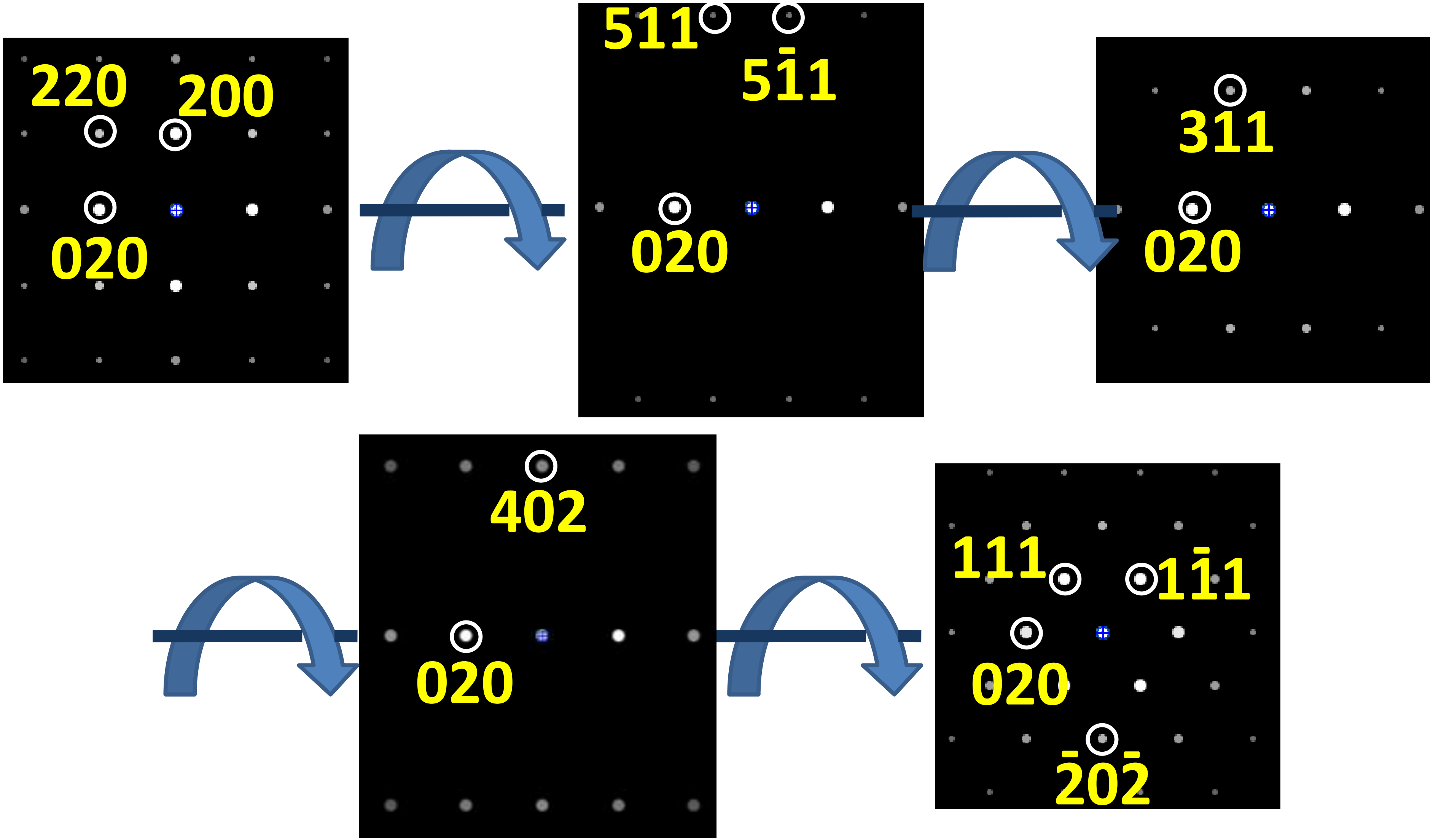
220
200
020
511
51̄1
020
311
020
0.91
020
2.34
2.34
020
1.43

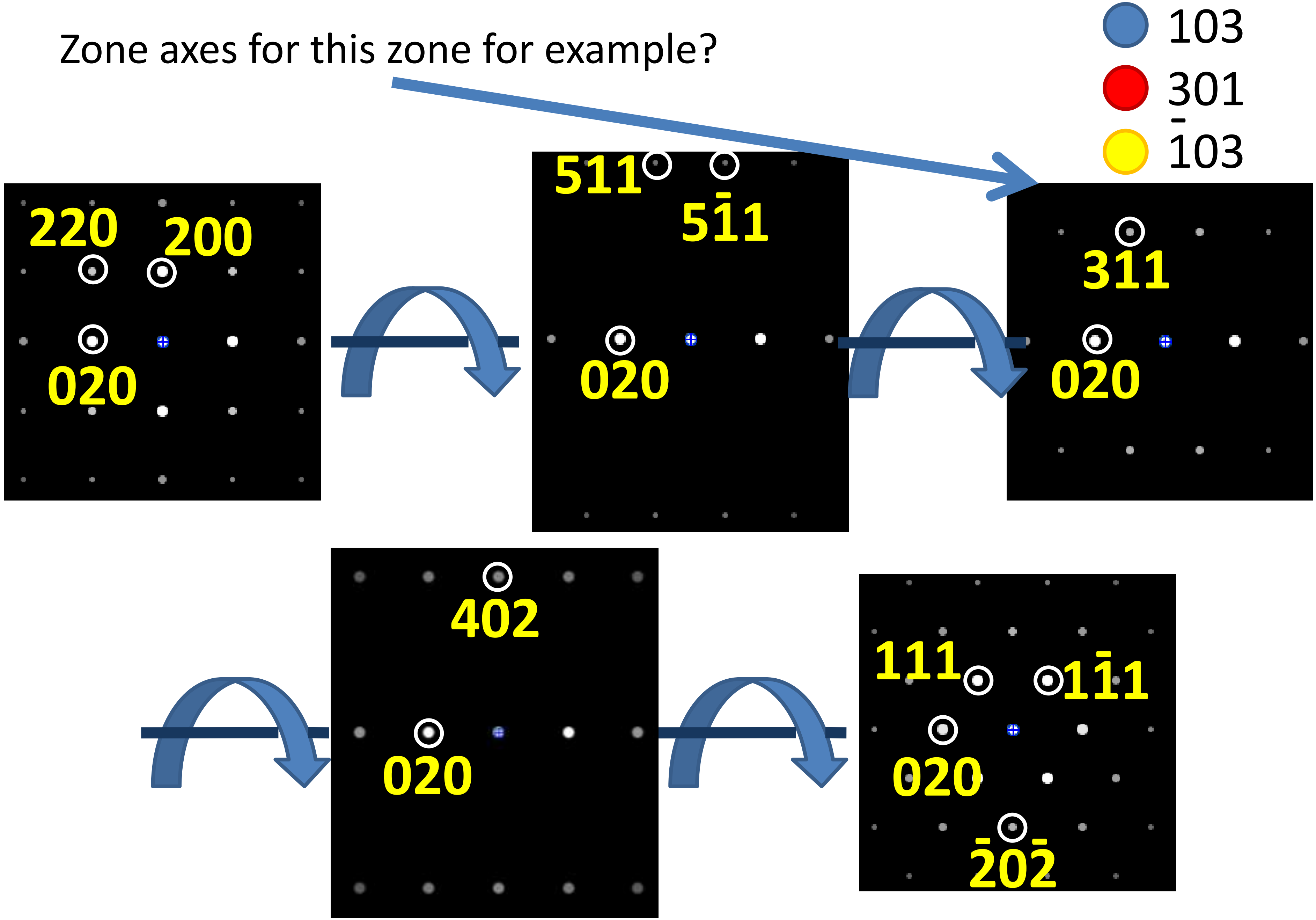


b*
a*
c*
100
200
300
400
500
001
101
201
301
401
501
002
102
202
302
402
502
003
103
203
303
403
503

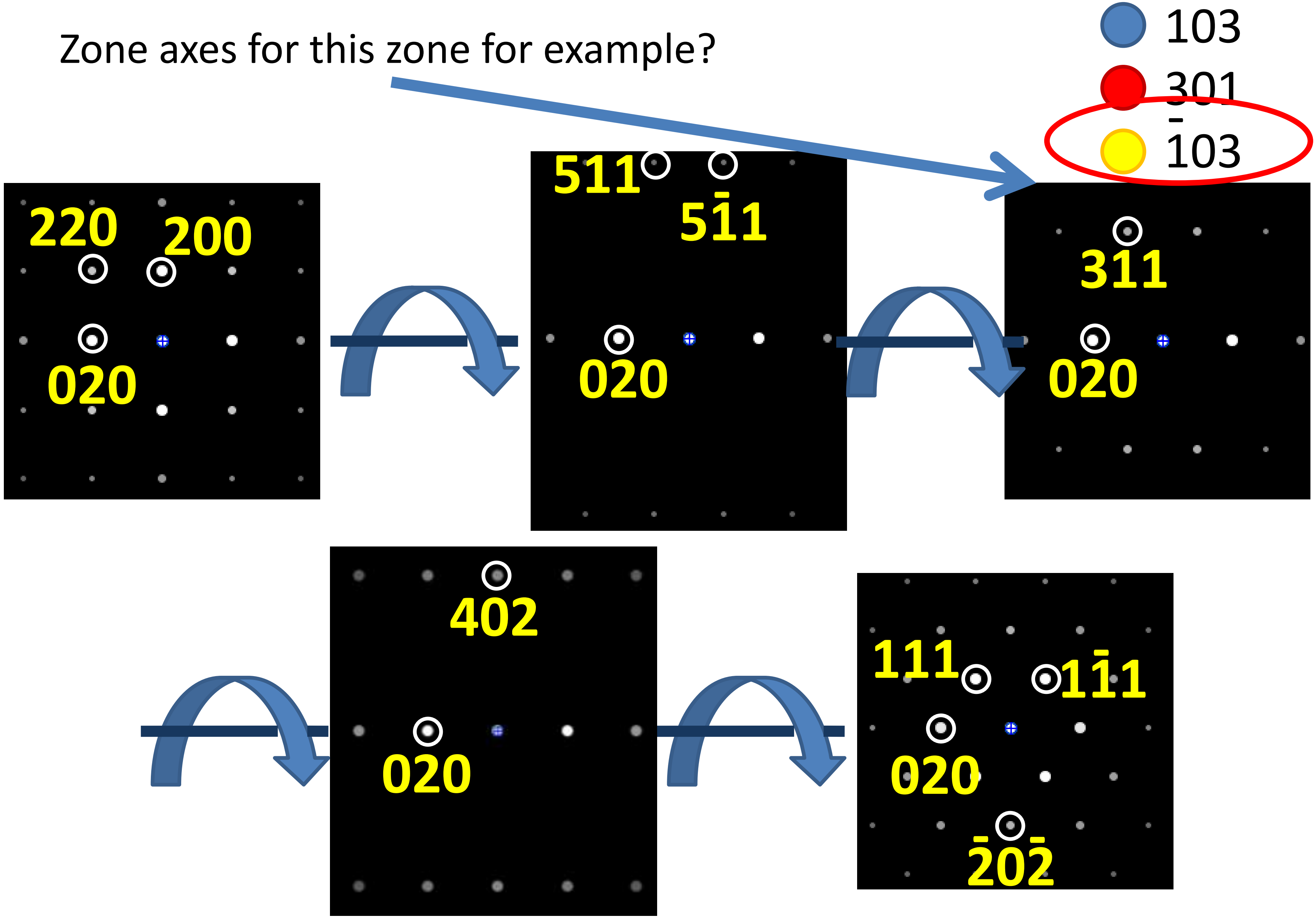

220
200
020
511
5̄11
020
311
020
402
020
2.34
2.34
020
1.43


220
200
020
511
5$\bar{1}$1
020
311
020
402
020
111
1$\bar{1}$1
020

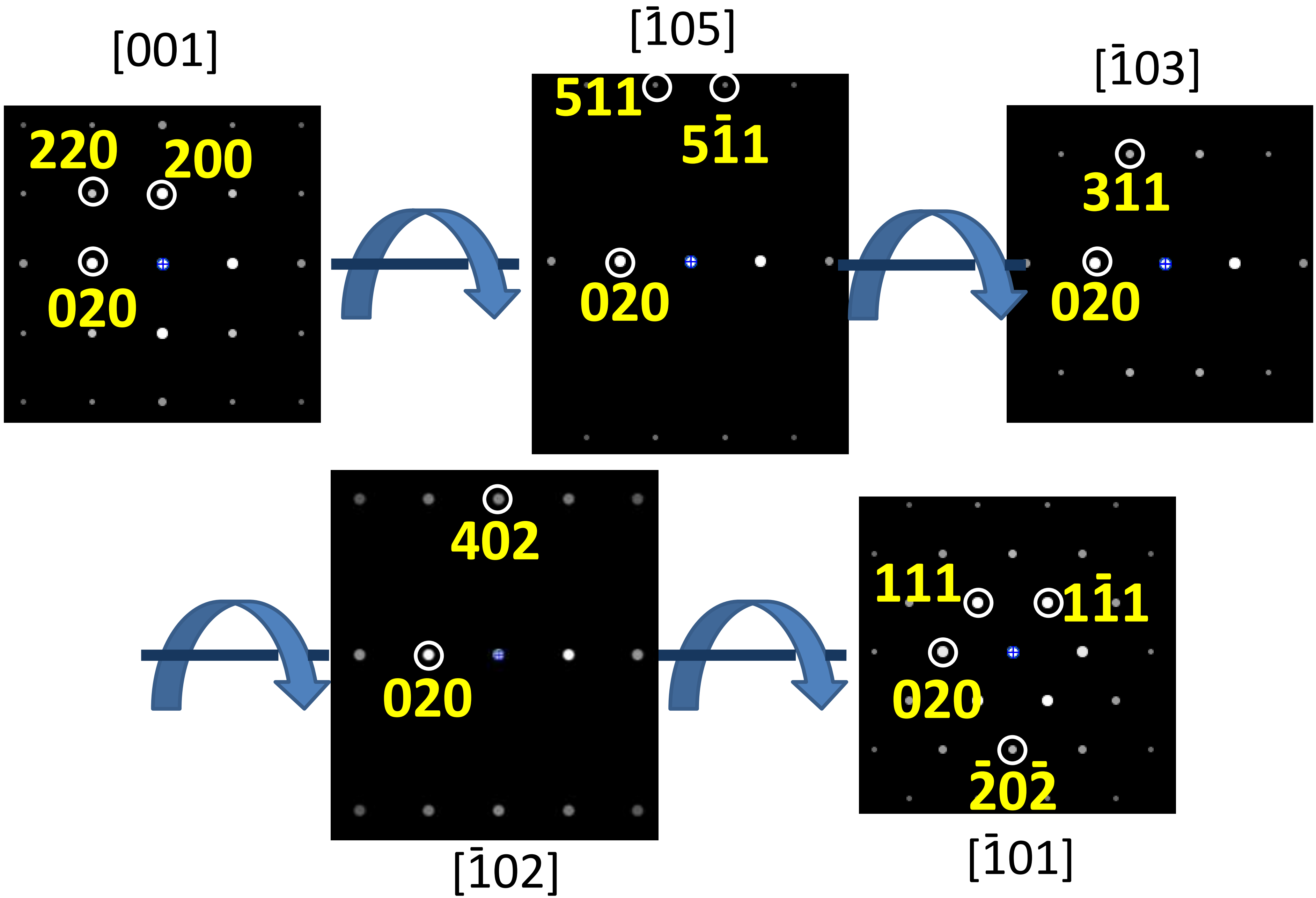

220
200
020
511
51̄1
020
311
020
402
020
111
11̄1
020
2̄02̄



Zone axes for this zone for example?
103
301
1̄03
220
200
020
511
51̄1
020
311
020
402
020
111
11̄1
020
2̄02̄



Zone axes for this zone for example?
103
301
$\bar{1}03$
220
200
020
511
$5\bar{1}1$
020
311
020
402
020
111
$1\bar{1}1$
020
$\bar{2}0\bar{2}$


[001]
220
200
020
[1̄05]
511
51̄1
020
[1̄03]
311
020
[1̄02]
402
020
[1̄01]
111
11̄1
020
2̄02̄

Indexed
-> cell parameter:
a=4.06 Å

Space group?
Possibility from SAED:
extinction symbol.
-> Determine reflection conditions.

Reflection conditions (Indices are permutable, apart from space group No. 205) ††				Extinction symbol	Point group				
hkl	$0kl$	hhl	$00l$		23	$m\bar{3}$	432	$\bar{4}3m$	$m\bar{3}m$
				$P---$	$P23$ (195)	$Pm\bar{3}$ (200)	$P432$ (207)	$P\bar{4}3m$ (215)	$Pm\bar{3}m$ (221)
			l	$\{P2_1--$, $P4_2--\}$	$P2_13$ (198)		$P4_232$ (208)		
			$l=4n$	$P4_1--$			$\{P4_132$ (213), $P4_332$ (212)$\}$ ‡‡		
		l	l	$P--n$				$P\bar{4}3n$ (218)	$Pm\bar{3}n$ (223)
	k††		l	$Pa--$		$Pa\bar{3}$ (205)			
	$k+l$		l	$Pn--$		$Pn\bar{3}$ (201)			$Pn\bar{3}m$ (224)
	$k+l$	l	l	$Pn-n$					$Pn\bar{3}n$ (222)
$h+k+l$	$k+l$	l	l	$I---$	$[I23$ (197), $I2_13$ (199)$]$ §§	$Im\bar{3}$ (204)	$I432$ (211)	$I\bar{4}3m$ (217)	$Im\bar{3}m$ (229)
$h+k+l$	$k+l$	l	$l=4n$	$I4_1--$			$I4_132$ (214)		
$h+k+l$	$k+l$	$2h+l=4n, l$	$l=4n$	$I--d$				$I\bar{4}3d$ (220)	
$h+k+l$	k, l	l	l	$Ia--$		$Ia\bar{3}$ (206)			
$h+k+l$	k, l	$2h+l=4n, l$	$l=4n$	$Ia-d$					$Ia\bar{3}d$ (230)
$h+k, h+l, k+l$	k, l	$h+l$	l	$F---$	$F23$ (196)	$Fm\bar{3}$ (202)	$F432$ (209)	$F\bar{4}3m$ (216)	$Fm\bar{3}m$ (225)
$h+k, h+l, k+l$	k, l	$h+l$	$l=4n$	$F4_1--$			$F4_132$ (210)		
$h+k, h+l, k+l$	k, l	h, l	l	$F--c$				$F\bar{4}3c$ (219)	$Fm\bar{3}c$ (226)
$h+k, h+l, k+l$	$k+l=4n, k, l$	$h+l$	$l=4n$	$Fd--$		$Fd\bar{3}$ (203)			$Fd\bar{3}m$ (227)
$h+k, h+l, k+l$	$k+l=4n, k, l$	h, l	$l=4n$	$Fd-c$					$Fd\bar{3}c$ (228)

hkl: (blue) h+k+l=2n

(red) all odd, all even

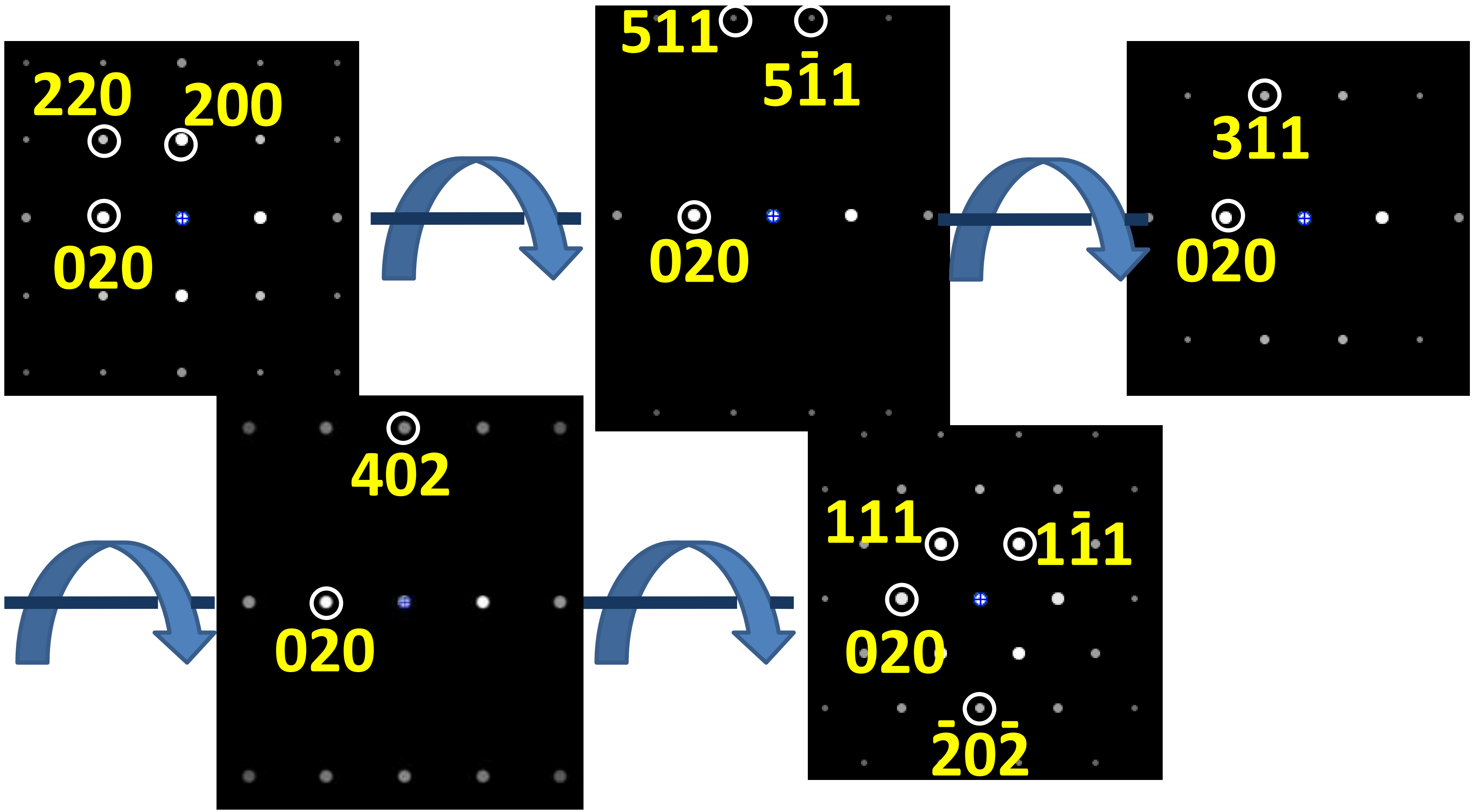
(yellow) no conditions

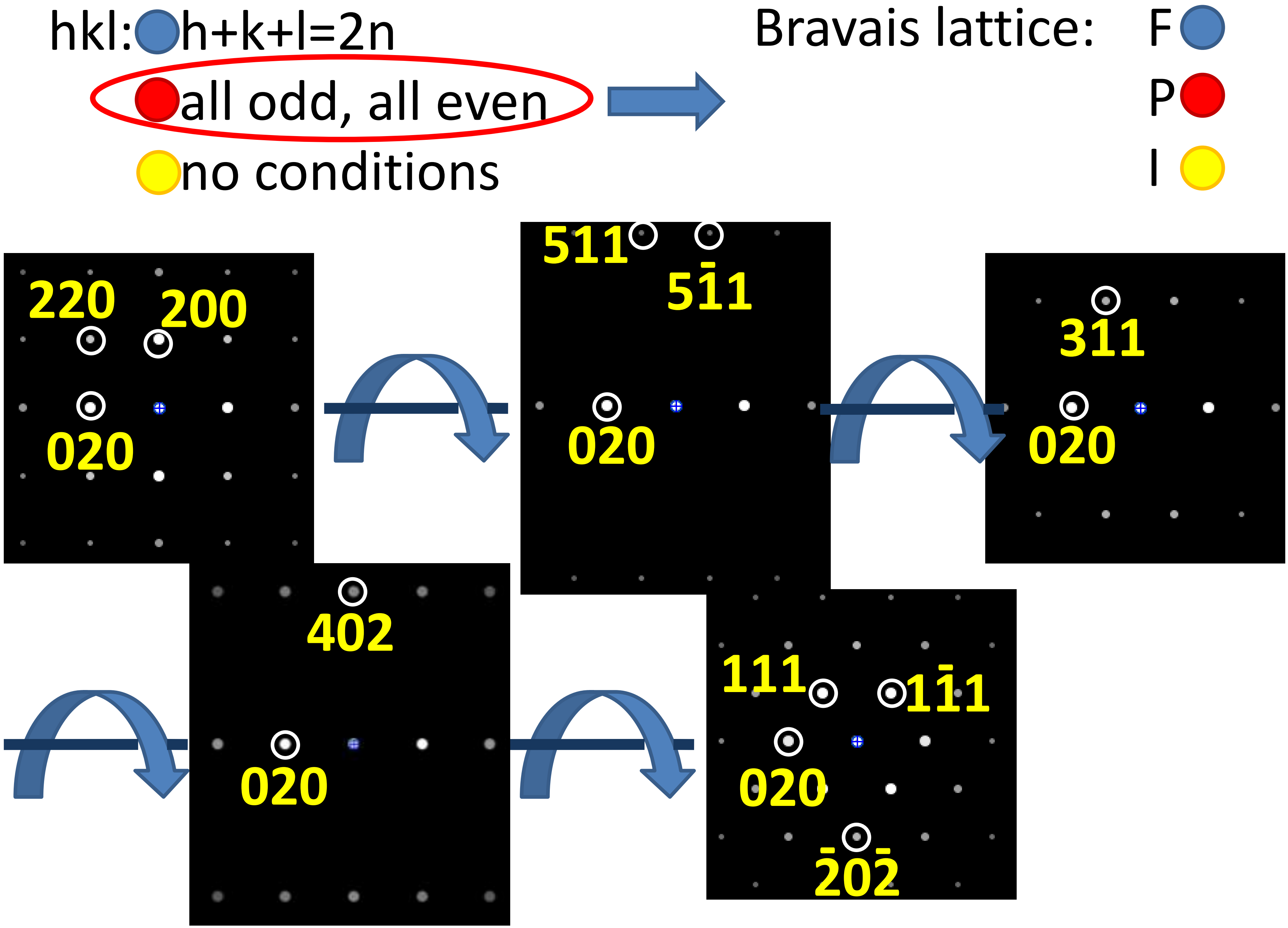
→

Bravais lattice: F (blue)

P (red)

I (yellow)




hkl: h+k+l=2n
all odd, all even
no conditions
Bravais lattice: F
P
I
220
200
020
511
$5\bar{1}1$
020
311
020
402
020
111
$1\bar{1}1$
020
$\bar{2}0\bar{2}$

hkl: h+k+l=2n

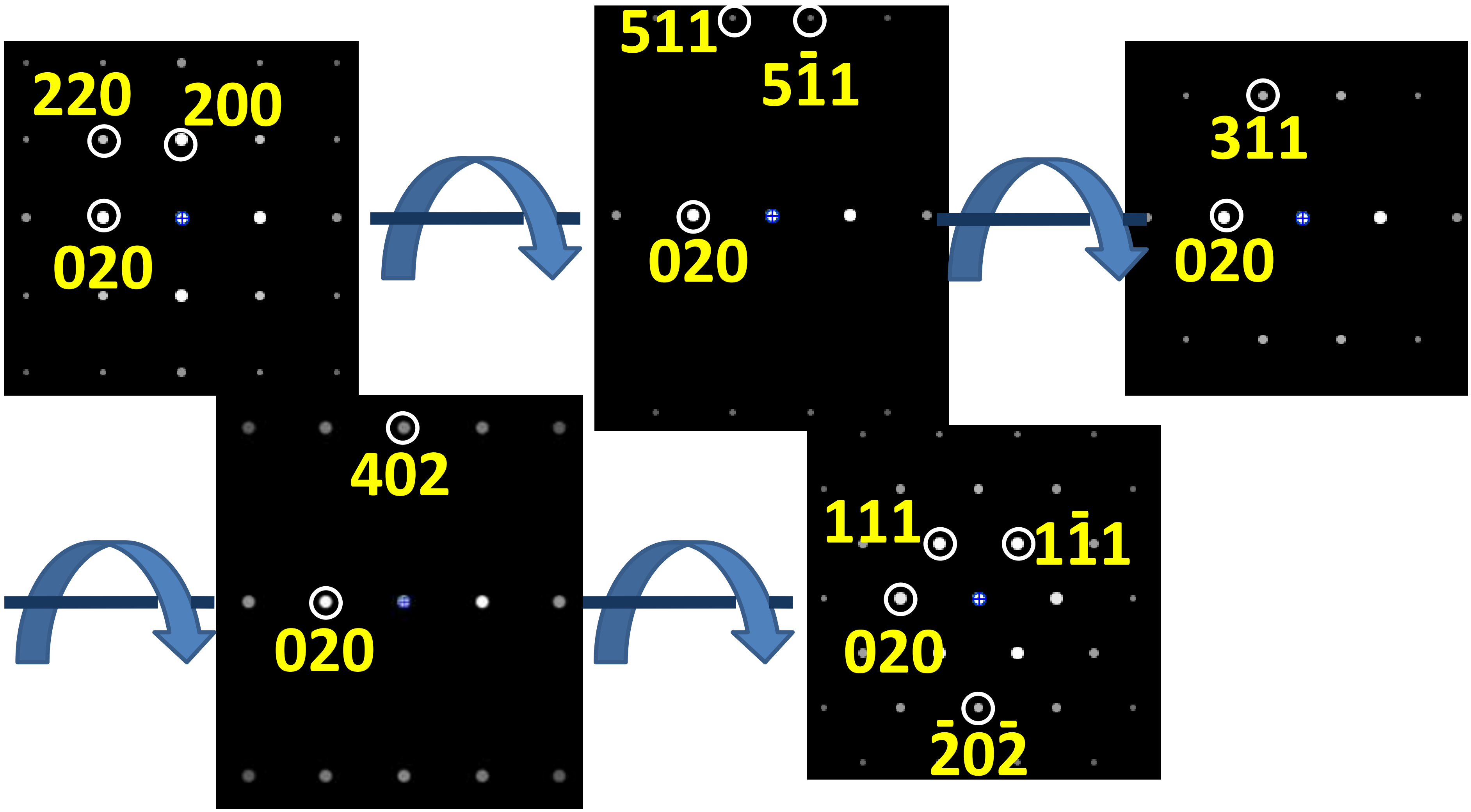
all odd, all even

no conditions

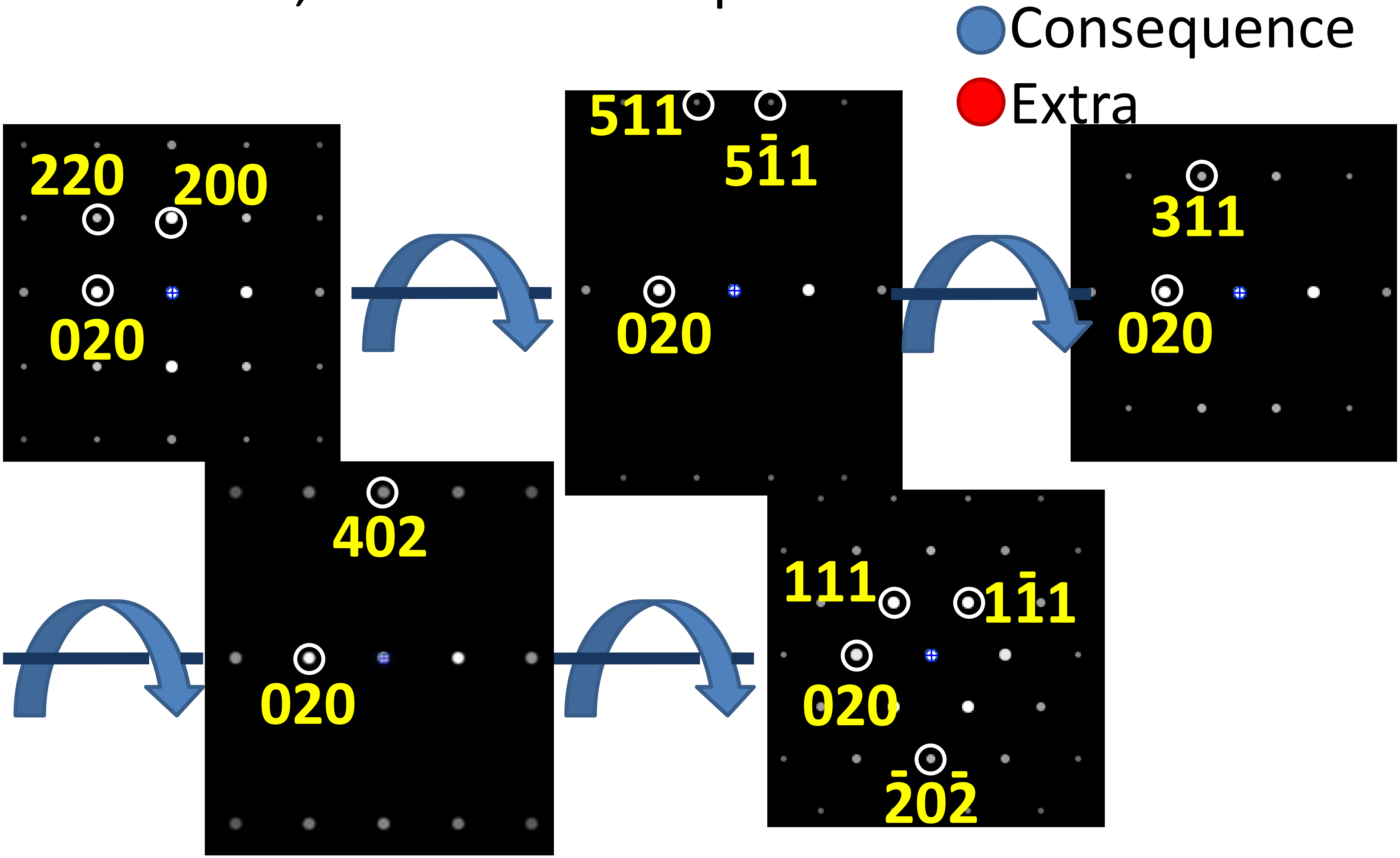
Bravais lattice: F

P

I

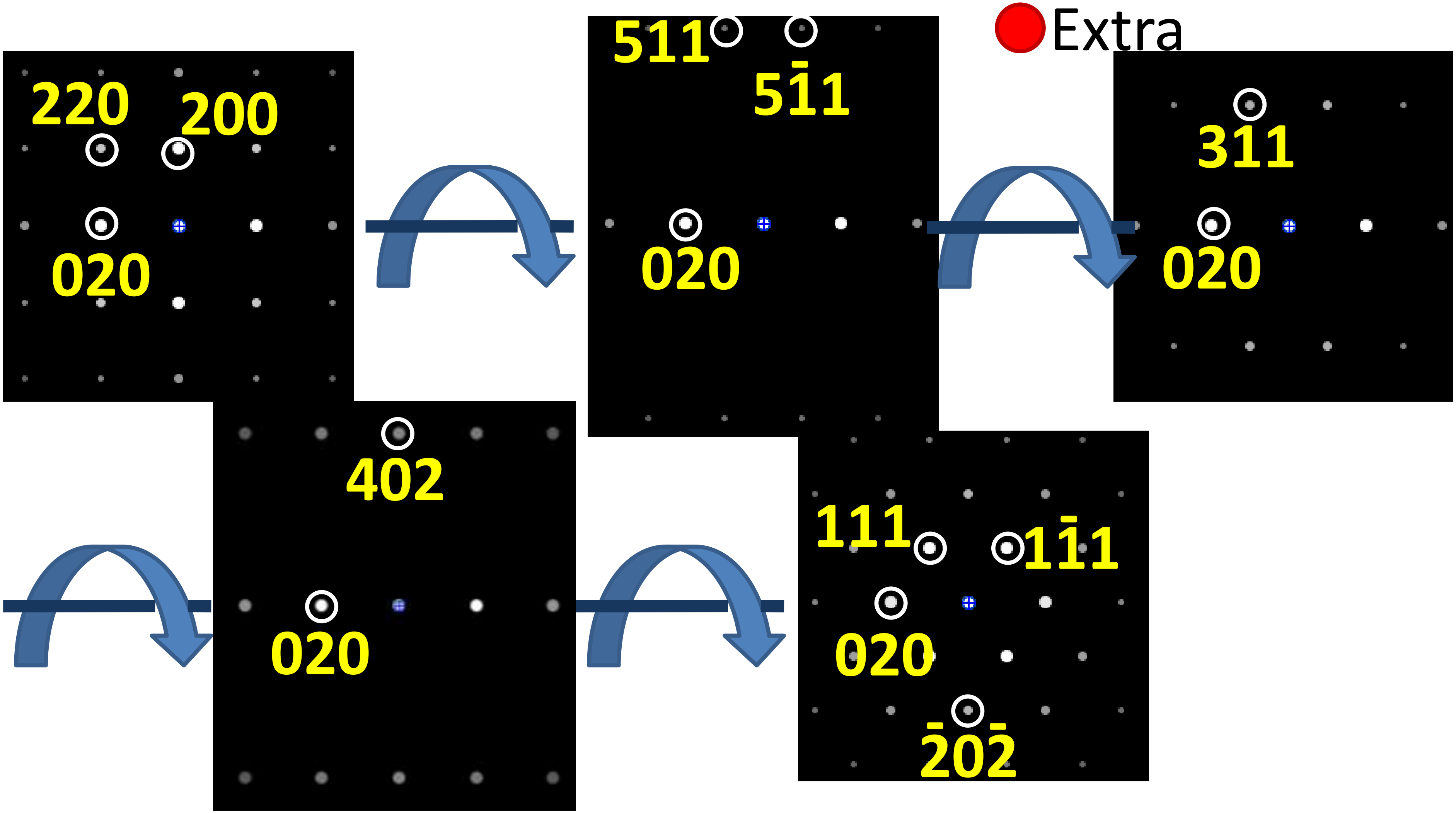


We know: hk0: h=2n, k=2n. Is this an extra condition, or is it a consequence of F also?



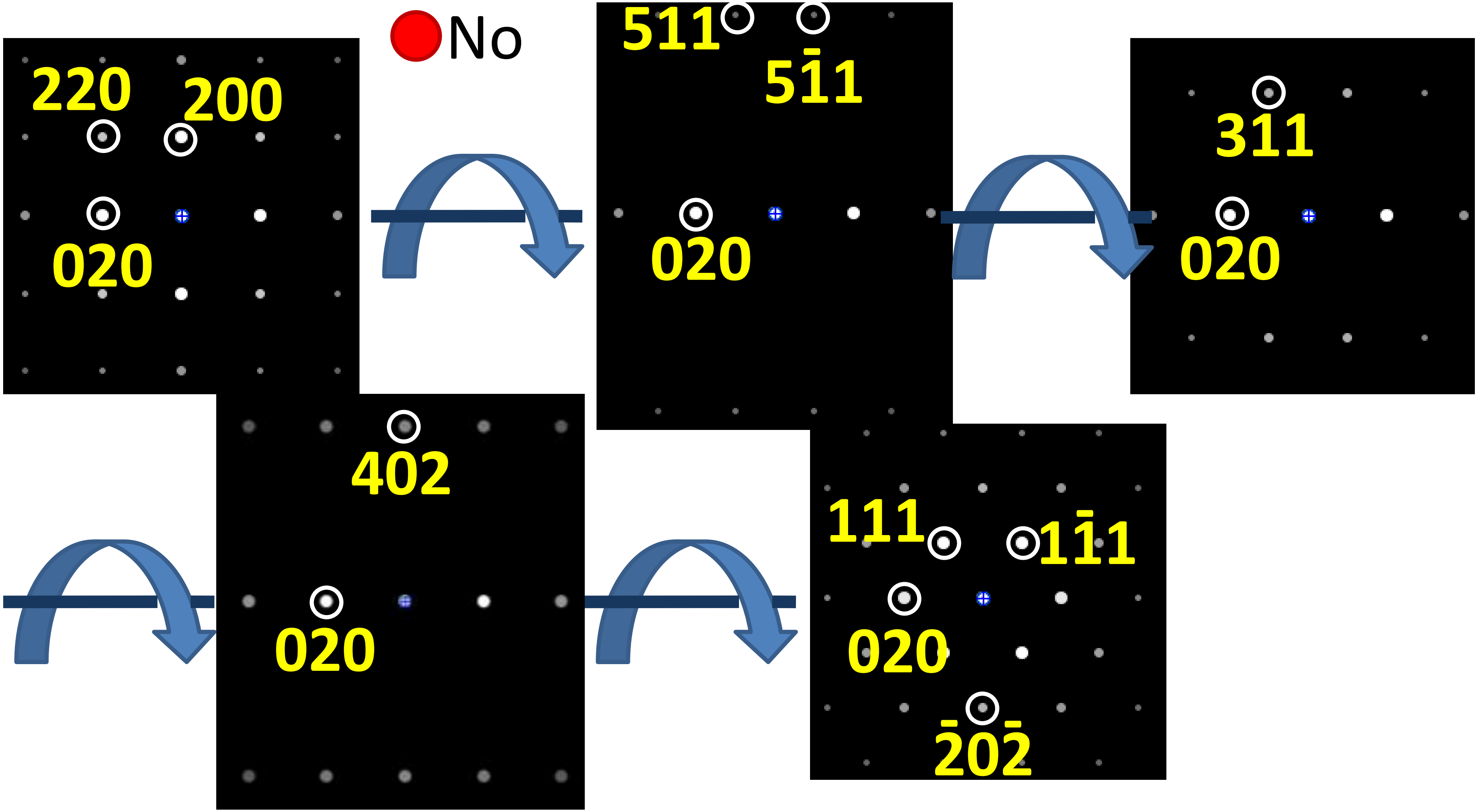
We know: hk0: h=2n, k=2n. Is this an extra condition, or is it a consequence of F also?

- Consequence
- Extra



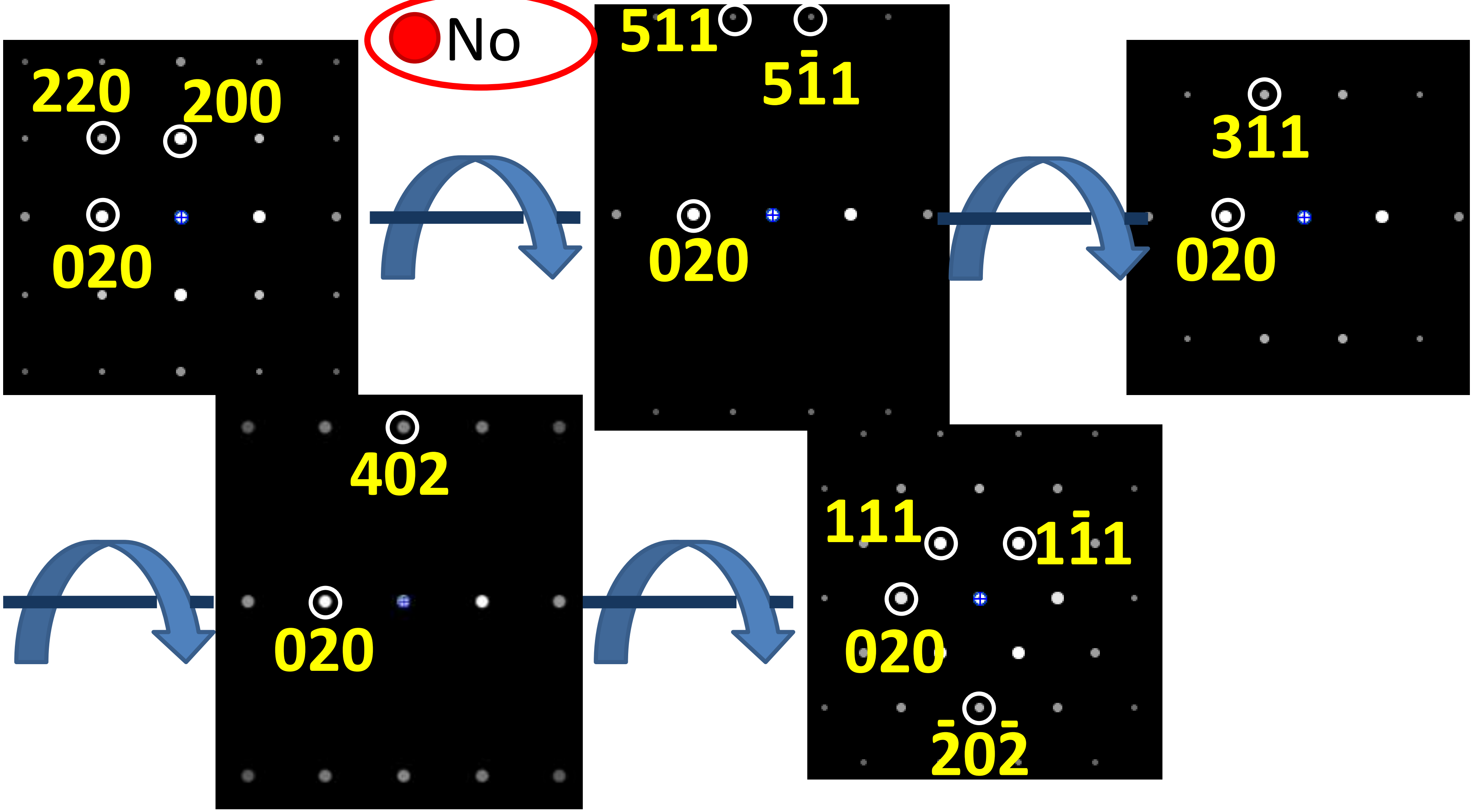
Are there ànу extra conditions, i.e. conditions that are not already implied by hkl: all odd, all even?

- Yes
- No



Are there ȁny extra conditions, i.e. conditions that are not already implied by hkl: all odd, all even?

- Yes
- No



Reflection conditions (Indices are permutable, apart from space group No. 205) ††				Extinction symbol	Laue class $m\bar{3}$ ($2/m\ \bar{3}$)		Laue class $m\bar{3}m$ ($4/m\ \bar{3}\ 2/m$)		
					Point group				
hkl	$0kl$	hhl	$00l$		23	$m\bar{3}$	432	$\bar{4}3m$	$m\bar{3}m$
				$P---$	$P23$ (195)	$Pm\bar{3}$ (200)	$P432$ (207)	$P\bar{4}3m$ (215)	$Pm\bar{3}m$ (221)
			l	$\{P2_1--$, $P4_2--\}$	$P2_13$ (198)		$P4_232$ (208)		
			$l=4n$	$P4_1--$			$\{P4_132$ (213), $P4_332$ (212)$\}$ ‡‡		
		l	l	$P--n$				$P\bar{4}3n$ (218)	$Pm\bar{3}n$ (223)
	k††		l	$Pa--$		$Pa\bar{3}$ (205)			
	$k+l$		l	$Pn--$		$Pn\bar{3}$ (201)			$Pn\bar{3}m$ (224)
	$k+l$	l	l	$Pn-n$					$Pn\bar{3}n$ (222)
$h+k+l$	$k+l$	l	l	$I---$	$[I23$ (197), $I2_13$ (199)$]$ §§	$Im\bar{3}$ (204)	$I432$ (211)	$I\bar{4}3m$ (217)	$Im\bar{3}m$ (229)
$h+k+l$	$k+l$	l	$l=4n$	$I4_1--$			$I4_132$ (214)		
$h+k+l$	$k+l$	$2h+l=4n, l$	$l=4n$	$I--d$				$I\bar{4}3d$ (220)	
$h+k+l$	k, l	l	l	$Ia--$		$Ia\bar{3}$ (206)			
$h+k+l$	k, l	$2h+l=4n, l$	$l=4n$	$Ia-d$					$Ia\bar{3}d$ (230)
$h+k, h+l, k+l$	k, l	$h+l$	l	$F---$	$F23$ (196)	$Fm\bar{3}$ (202)	$F432$ (209)	$F\bar{4}3m$ (216)	$Fm\bar{3}m$ (225)
$h+k, h+l, k+l$	k, l	$h+l$	$l=4n$	$F4_1--$			$F4_132$ (210)		
$h+k, h+l, k+l$	k, l	h, l	l	$F--c$				$F\bar{4}3c$ (219)	$Fm\bar{3}c$ (226)
$h+k, h+l, k+l$	$k+l=4n, k, l$	$h+l$	$l=4n$	$Fd--$		$Fd\bar{3}$ (203)			$Fd\bar{3}m$ (227)
$h+k, h+l, k+l$	$k+l=4n, k, l$	h, l	$l=4n$	$Fd-c$					$Fd\bar{3}c$ (228)

Possible space groups: F23, Fm$\bar{3}$, F432, F$\bar{4}$3m, Fm$\bar{3}$m

from: International Tables for Crystallography Volume A, ed. Theo Hahn, Kluwer Ac. Pub., 2002

Possible space groups: F23, $Fm\bar{3}$, F432, $F\bar{4}3m$, $Fm\bar{3}m$

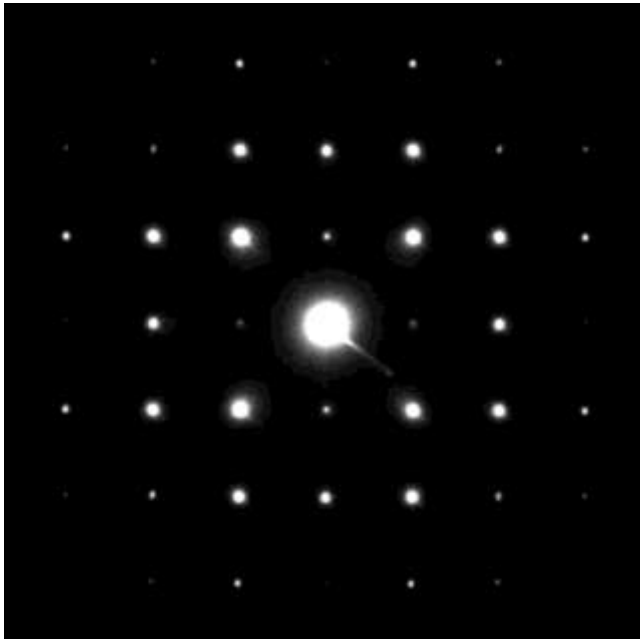
Same extinctions.

Difference: $\bar{1}$, 2, m; give no extinctions.

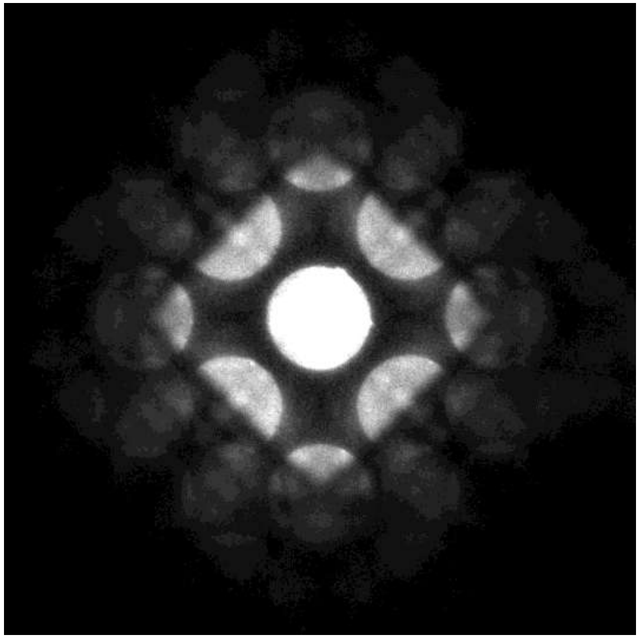
Convergent beam electron diffraction

CBED

2. Convergent beam electron diffraction (CBED)



SAED



CBED

Example: rutile-type SnO_2

Projection symmetry: 2D, diffuse features

Full symmetry: 3D, sharp features

BF

WP

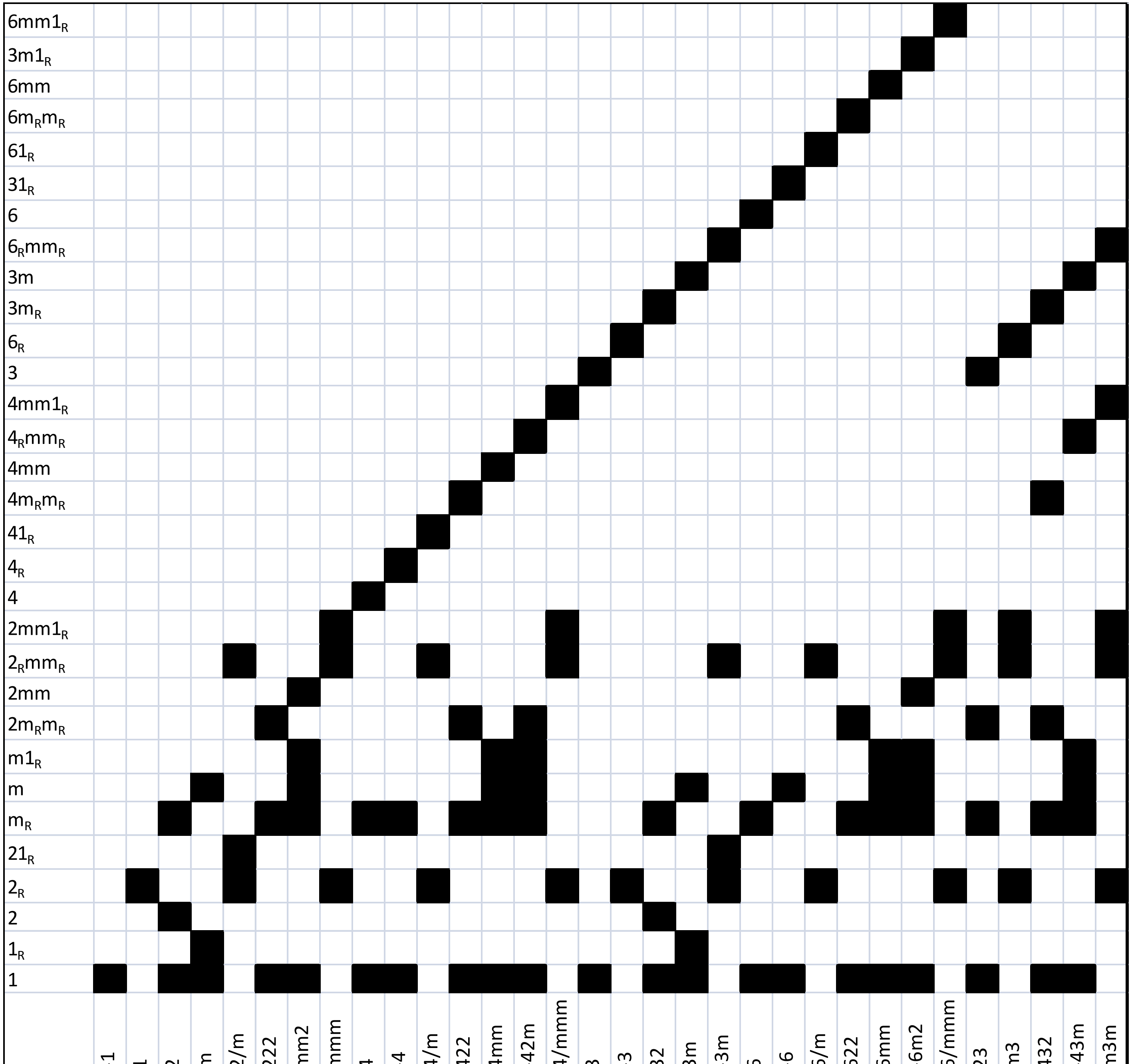
Lots of tables!

Point groups vs. diffraction groups

Table (b) Relation between diffraction groups and crystal point-groups

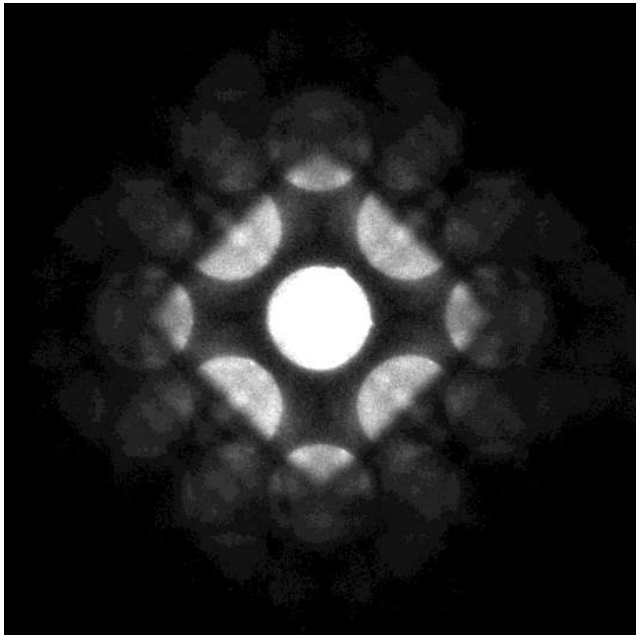
	1	$\bar{1}$	2	m	$2/m$	222	$mm2$	mmm	4	$\bar{4}$	$4/m$	422	$4mm$	$\bar{4}2m$	$4/mmm$	3	$\bar{3}$	32	$3m$	$\bar{3}m$	6	$\bar{6}$	$6/m$	622	$6mm$	$\bar{6}m2$	$6/mmm$	23	$m3$	432	$\bar{4}3m$	$m3m$
$6mm1_R$																											○					
$3m1_R$																										○						
$6mm$																									○							
$6m_Rm_R$																								○								
61_R																							○									
31_R																						○										
6																					○											
6_Rmm_R																				○												○
$3m$																			○												○	
$3m_R$																		○												○		
6_R																	○												○			
3																○												○				
$4mm1_R$															○																	○
4_Rmm_R														○																	○	
$4mm$													○																			
$4m_Rm_R$												○																		○		
41_R											○																					
4_R										○																						
4									○																							
$2mm1_R$								○							○												○		○			○
2_Rmm_R					○			○			○				○					○			○				○		○			○
$2mm$							○																			○						
$2m_Rm_R$						○						○		○										○				○		○		
$m1_R$							○						○	○											○	○					○	
m				○			○						○	○					○			○			○	○					○	
m_R			○			○	○		○	○		○	○	○				○			○			○	○	○		○		○	○	
21_R					○															○												
2_R		○			○			○			○				○		○			○			○				○		○			○
2			○															○														
1_R				○															○													
1	○		○	○		○	○		○	○		○	○	○		○		○	○		○	○		○	○	○		○		○	○	

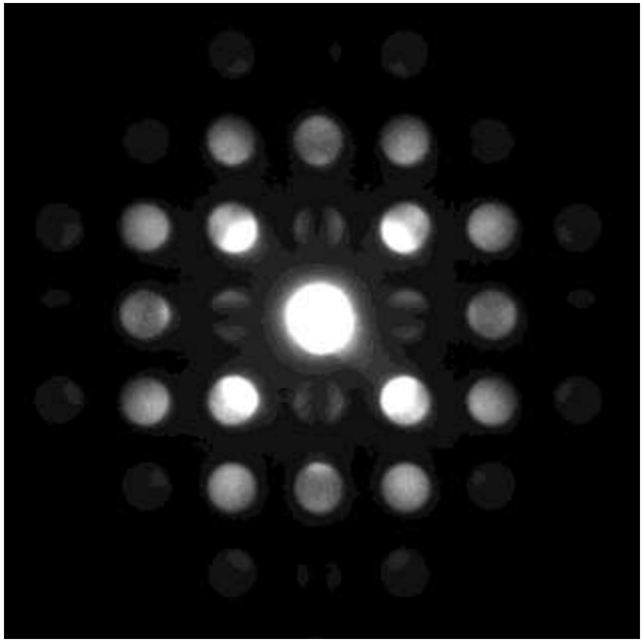
B.F. Buxton, J.A. Eades, J.W. Steeds and G.M. Rackham: *Phil. Trans. R. Soc. London*, **281** (1976) 171.
Courtesy of the Royal Society of London



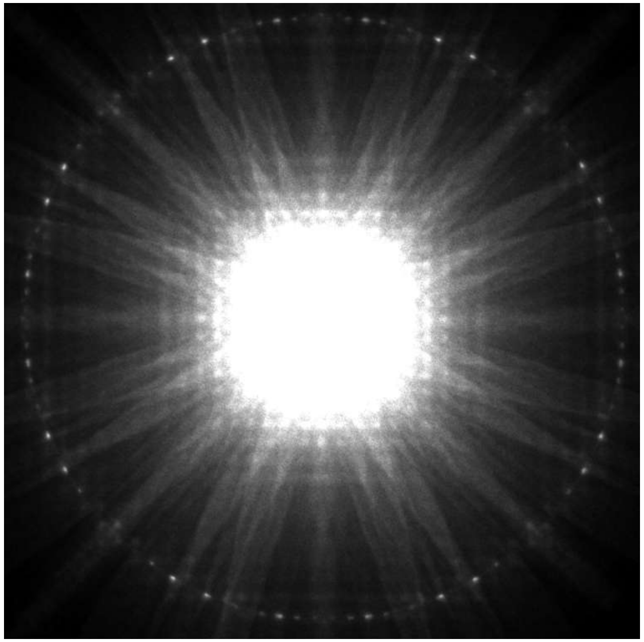
6mm1$_R$
3m1$_R$
6mm
6m$_R$m$_R$
61$_R$
31$_R$
6
6$_R$mm$_R$
3m
3m$_R$
6$_R$
3
4mm1$_R$
4$_R$mm$_R$
4mm
4m$_R$m$_R$
41$_R$
4$_R$
4
2mm1$_R$
2$_R$mm$_R$
2mm
2m$_R$m$_R$
m1$_R$
m
m$_R$
21$_R$
2$_R$
2
1$_R$
1
-1
1
2
m
2/m
222
mm2
mmm
4
-4
4/m
422
4mm
-42m
4/mmm
3
-3
32
3m
-3m
6
-6
6/m
622
6mm
-6m2
6/mmm
23
m3
432
-43m
m3m

WP proj

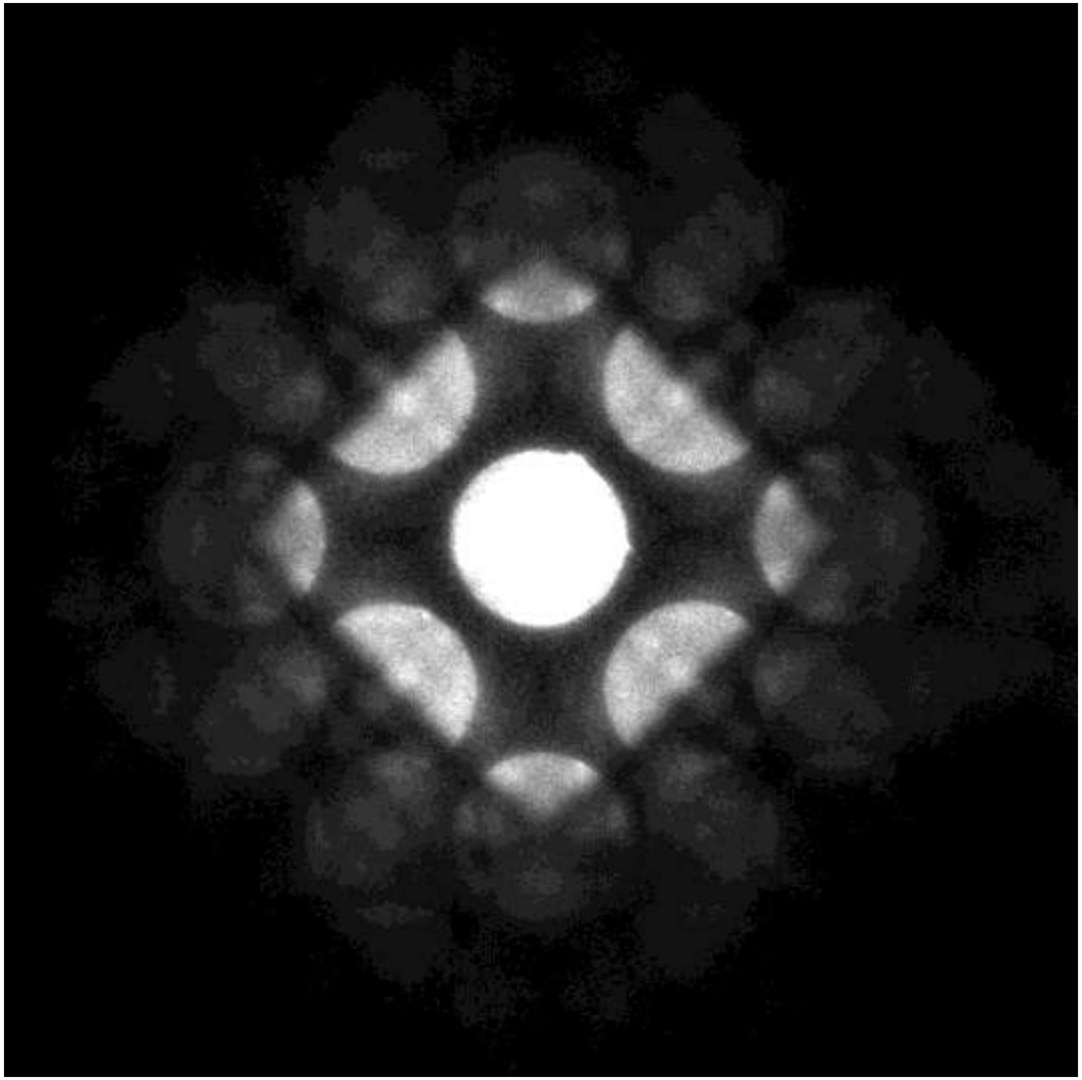




WP

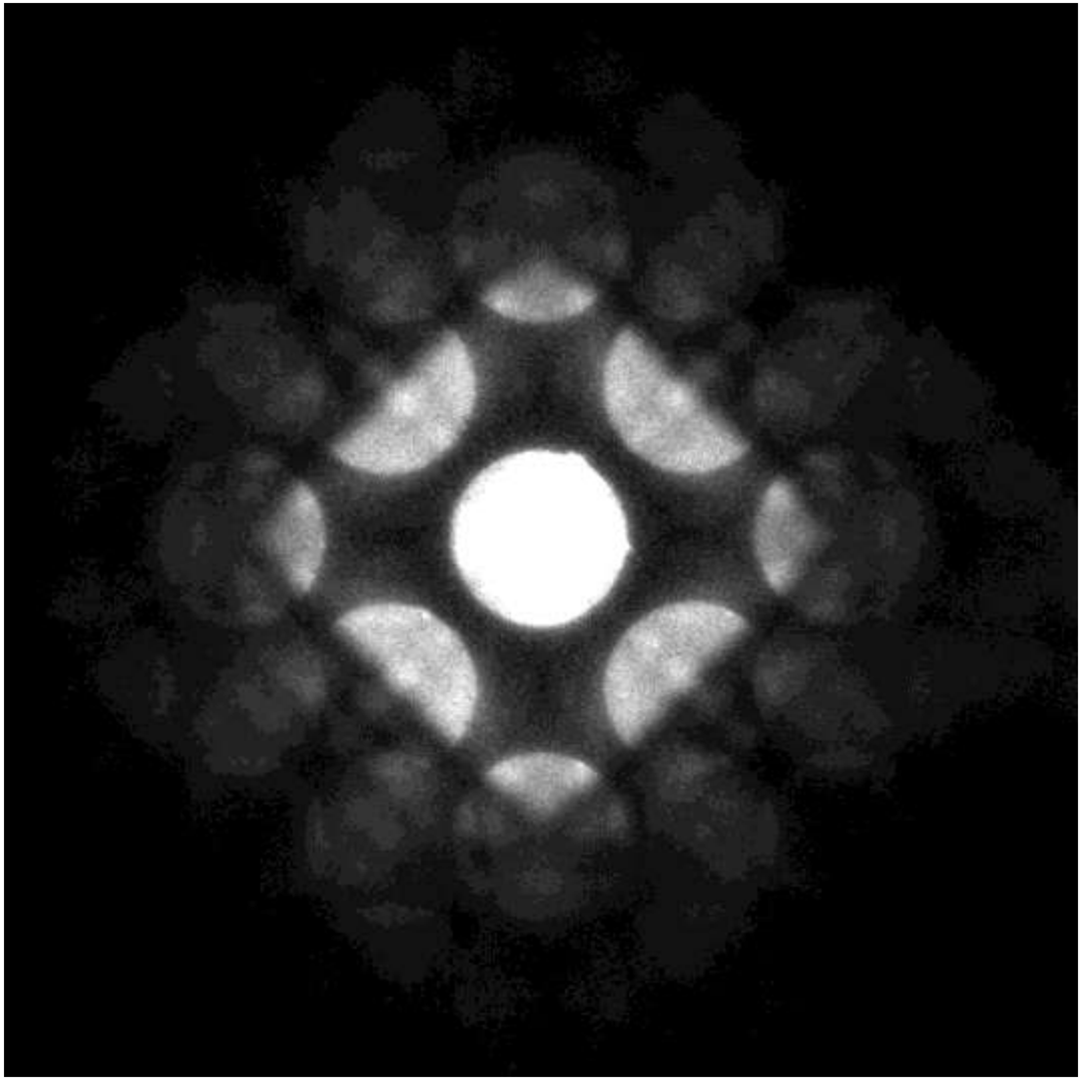


Projection whole pattern symmetry [001]



- 4
- 4mm
- 2mm

Projection whole pattern symmetry [001]



- 4
- 4mm
- 2mm

Projection WP: 4mm

Projection diffraction group: Table Eades

- 4
- 4_Rmm_R
- $4mm1_R$

Table 7.1: Diffraction Groups and Pattern Symmetries | **Table 7.2: Projection Diffraction Groups and Pattern Symmetries**

diffraction group	bright field	whole pattern	projection diffraction group	projection diffraction group	bright field	whole pattern
1	1	1	1_R	1_R	2	1
1_R	2	1	1_R			
2	2	2	21_R	21_R	2	2
2_R	1	1	21_R			
21_R	2	2	21_R			
m_R	m	1	$m1_R$	$m1_R$	2mm	m
m	m	m	$m1_R$			
$m1_R$	2mm	m	$m1_R$			
$2m_Rm_R$	2mm	2	$2mm1_R$	$2mm1_R$	2mm	2mm
2mm	2mm	2mm	$2mm1_R$			
2_Rmm_R	m	m	$2mm1_R$			
$2mm1_R$	2mm	2mm	$2mm1_R$			
4	4	4	41_R	41_R	4	4
4_R	4	2	41_R			
41_R	4	4	41_R			
$4m_Rm_R$	4mm	4	$4mm1_R$	$4mm1_R$	4mm	4mm
4mm	4mm	4mm	$4mm1_R$			
4_Rmm_R	4mm	2mm	$4mm1_R$			
$4mm1_R$	4mm	4mm	$4mm1_R$			
3	3	3	31_R	31_R	6	3
31_R	6	3	31_R			
$3m_R$	3m	3	$3m1_R$	$3m1_R$	6mm	3m
3m	3m	3m	$3m1_R$			
$3m1_R$	6mm	3m	$3m1_R$			
6	6	6	61_R	61_R	6	6
6_R	3	3	61_R			
61_R	6	6	61_R			
$6m_Rm_R$	6mm	6	$6mm1_R$	$6mm1_R$	6mm	6mm
6mm	6mm	6mm	$6mm1_R$			
6_Rmm_R	3m	3m	$6mm1_R$			
$6mm1_R$	6mm	6mm	$6mm1_R$			

Table from: J.A. Eades, Convergent beam diffraction, in: Electron Diffraction Techniques, volume 1, ed. J. Cowley, Oxford University Press, 1992

Projection WP: 4mm

Projection diffraction group:
Table Eades

- 4
- 4_Rmm_R
- $4mm1_R$

Table 7.1: Diffraction Groups and Pattern Symmetries

diffraction group	bright field	whole pattern	projection diffraction group
1	1	1	1_R
1_R	2	1	1_R
2	2	2	21_R
2_R	1	1	21_R
21_R	2	2	21_R
m_R	m	1	$m1_R$
m	m	m	$m1_R$
$m1_R$	2mm	m	$m1_R$
$2m_Rm_R$	2mm	2	$2mm1_R$
2mm	2mm	2mm	$2mm1_R$
2_Rmm_R	m	m	$2mm1_R$
$2mm1_R$	2mm	2mm	$2mm1_R$
4	4	4	41_R
4_R	4	2	41_R
41_R	4	4	41_R
$4m_Rm_R$	4mm	4	$4mm1_R$
4mm	4mm	4mm	$4mm1_R$
4_Rmm_R	4mm	2mm	$4mm1_R$
$4mm1_R$	4mm	4mm	$4mm1_R$
3	3	3	31_R
31_R	6	3	31_R
$3m_R$	3m	3	$3m1_R$
3m	3m	3m	$3m1_R$
$3m1_R$	6mm	3m	$3m1_R$
6	6	6	61_R
6_R	3	3	61_R
61_R	6	6	61_R
$6m_Rm_R$	6mm	6	$6mm1_R$
6mm	6mm	6mm	$6mm1_R$
6_Rmm_R	3m	3m	$6mm1_R$
$6mm1_R$	6mm	6mm	$6mm1_R$

Table 7.2: Projection Diffraction Groups and Pattern Symmetries

projection diffraction group	bright field	whole pattern
1_R	2	1
21_R	2	2
$m1_R$	2mm	m
$2mm1_R$	2mm	2mm
41_R	4	4
$4mm1_R$	4mm	4mm
31_R	6	3
$3m1_R$	6mm	3m
61_R	6	6
$6mm1_R$	6mm	6mm

Table from: J.A. Eades, Convergent beam diffraction, in: Electron Diffraction Techniques, volume 1, ed. J. Cowley, Oxford University Press, 1992

Projection diffraction group:

$4mm1_R$

Possible diffraction groups:

$4m_Rm_R$

$4mm$

$4Rmm_R$

$4mm1_R$

Table 7.1: Diffraction Groups and Pattern Symmetries

diffraction group	bright field	whole pattern	projection diffraction group
1	1	1	1_R
1_R	2	1	1_R
2	2	2	21_R
2_R	1	1	21_R
21_R	2	2	21_R
m_R	m	1	$m1_R$
m	m	m	$m1_R$
$m1_R$	$2mm$	m	$m1_R$
$2m_Rm_R$	$2mm$	2	$2mm1_R$
$2mm$	$2mm$	$2mm$	$2mm1_R$
2_Rmm_R	m	m	$2mm1_R$
$2mm1_R$	$2mm$	$2mm$	$2mm1_R$
4	4	4	41_R
4_R	4	2	41_R
41_R	4	4	41_R
$4m_Rm_R$	$4mm$	4	$4mm1_R$
$4mm$	$4mm$	$4mm$	$4mm1_R$
4_Rmm_R	$4mm$	$2mm$	$4mm1_R$
$4mm1_R$	$4mm$	$4mm$	$4mm1_R$
3	3	3	31_R
31_R	6	3	31_R
$3m_R$	$3m$	3	$3m1_R$
$3m$	$3m$	$3m$	$3m1_R$
$3m1_R$	$6mm$	$3m$	$3m1_R$
6	6	6	61_R
6_R	3	3	61_R
61_R	6	6	61_R
$6m_Rm_R$	$6mm$	6	$6mm1_R$
$6mm$	$6mm$	$6mm$	$6mm1_R$
6_Rmm_R	$3m$	$3m$	$6mm1_R$
$6mm1_R$	$6mm$	$6mm$	$6mm1_R$

Table 7.2: Projection Diffraction Groups and Pattern Symmetries

projection diffraction group	bright field	whole pattern
1_R	2	1
21_R	2	2
$m1_R$	$2mm$	m
$2mm1_R$	$2mm$	$2mm$
41_R	4	4
$4mm1_R$	$4mm$	$4mm$
31_R	6	3
$3m1_R$	$6mm$	$3m$
61_R	6	6
$6mm1_R$	$6mm$	$6mm$

Table from: J.A. Eades, Convergent beam diffraction, in: Electron Diffraction Techniques, volume 1, ed. J. Cowley, Oxford University Press, 1992

	-1	1	2	m	2/m	222	mm2	mmm	4	-4	4/m	422	4mm	-42m	4/mmm	3	-3	32	3m	-3m	6	-6	6/m	622	6mm	-6m2	6/mmm	23	m3	432	-43m	m3m
$6mm1_R$																											■					
$3m1_R$																										■						
$6mm$																									■							
$6m_Rm_R$																								■								
61_R																							■									
31_R																						■										
6																					■											
6_Rmm_R																				■												■
$3m$																			■												■	
$3m_R$																		■												■		
6_R																	■												■			
3																■												■				
$4mm1_R$															■																	■
4_Rmm_R														■																	■	
$4mm$													■																			
$4m_Rm_R$												■																		■		
41_R											■																					
4_R										■																						
4									■																							
$2mm1_R$								■							■												■		■			■
2_Rmm_R					■			■			■				■					■			■				■		■			■
$2mm$							■																			■						
$2m_Rm_R$						■						■		■										■				■		■		
$m1_R$							■						■	■											■	■					■	
m				■			■						■	■					■			■			■	■					■	
m_R			■			■	■		■	■		■	■	■				■			■			■	■	■		■		■	■	
21_R					■															■												
2_R		■			■			■			■				■		■			■			■				■		■			■
2			■															■														
1_R				■															■													
1	■		■	■		■	■		■	■		■	■	■		■		■	■		■	■		■	■	■		■		■	■	

Table redrawn from B.F. Buxton, J.A. Eades, J.W. Steeds, G.M. Rackham: Phil. Trans. R. Soc. London, 281 (1976) 171

Table 7.1: Diffraction Groups and Pattern Symmetries

diffraction group	bright field	whole pattern	projection diffraction group
1	1	1	1_R
1_R	2	1	1_R
[...]			
4	4	4	41_R
4_R	4	2	41_R
41_R	4	4	41_R
$4m_Rm_R$	4mm	4	$4mm1_R$
4mm	4mm	4mm	$4mm1_R$
4_Rmm_R	4mm	2mm	$4mm1_R$
$4mm1_R$	4mm	4mm	$4mm1_R$

Table 7.2: Projection Diffraction Groups and Pattern Symmetries

projection diffraction group	bright field	whole pattern
1_R	2	1
[...]		
41_R	4	4
$4mm1_R$	4mm	4mm

What will be useful to narrow it down further?

- look at the bright field symmetry
- look at the whole pattern symmetry

Table 7.1: Diffraction Groups and Pattern Symmetries

diffraction group	bright field	whole pattern	projection diffraction group
1	1	1	1_R
1_R	2	1	1_R
[...]			
4	4	4	41_R
4_R	4	2	41_R
41_R	4	4	41_R
$4m_Rm_R$	4mm	4	$4mm1_R$
4mm	4mm	4mm	$4mm1_R$
4_Rmm_R	4mm	2mm	$4mm1_R$
$4mm1_R$	4mm	4mm	$4mm1_R$

Table 7.2: Projection Diffraction Groups and Pattern Symmetries

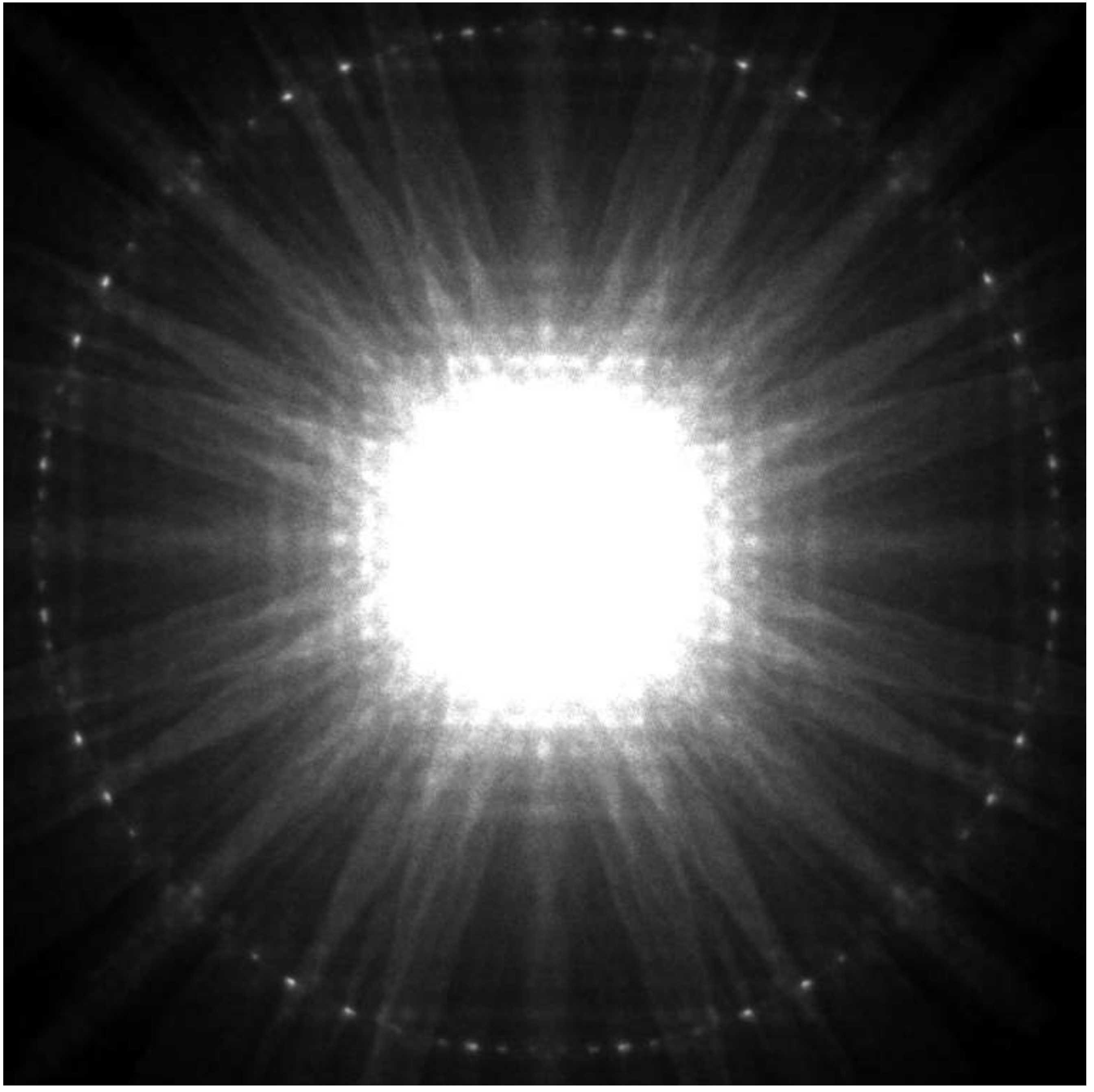
projection diffraction group	bright field	whole pattern
1_R	2	1
[...]		
41_R	4	4
$4mm1_R$	4mm	4mm

What will be useful to narrow it down further?

- look at the bright field symmetry
- look at the whole pattern symmetry

WP symmetry

4
4mm
2mm



WP symmetry

- 4
- 4mm
- 2mm

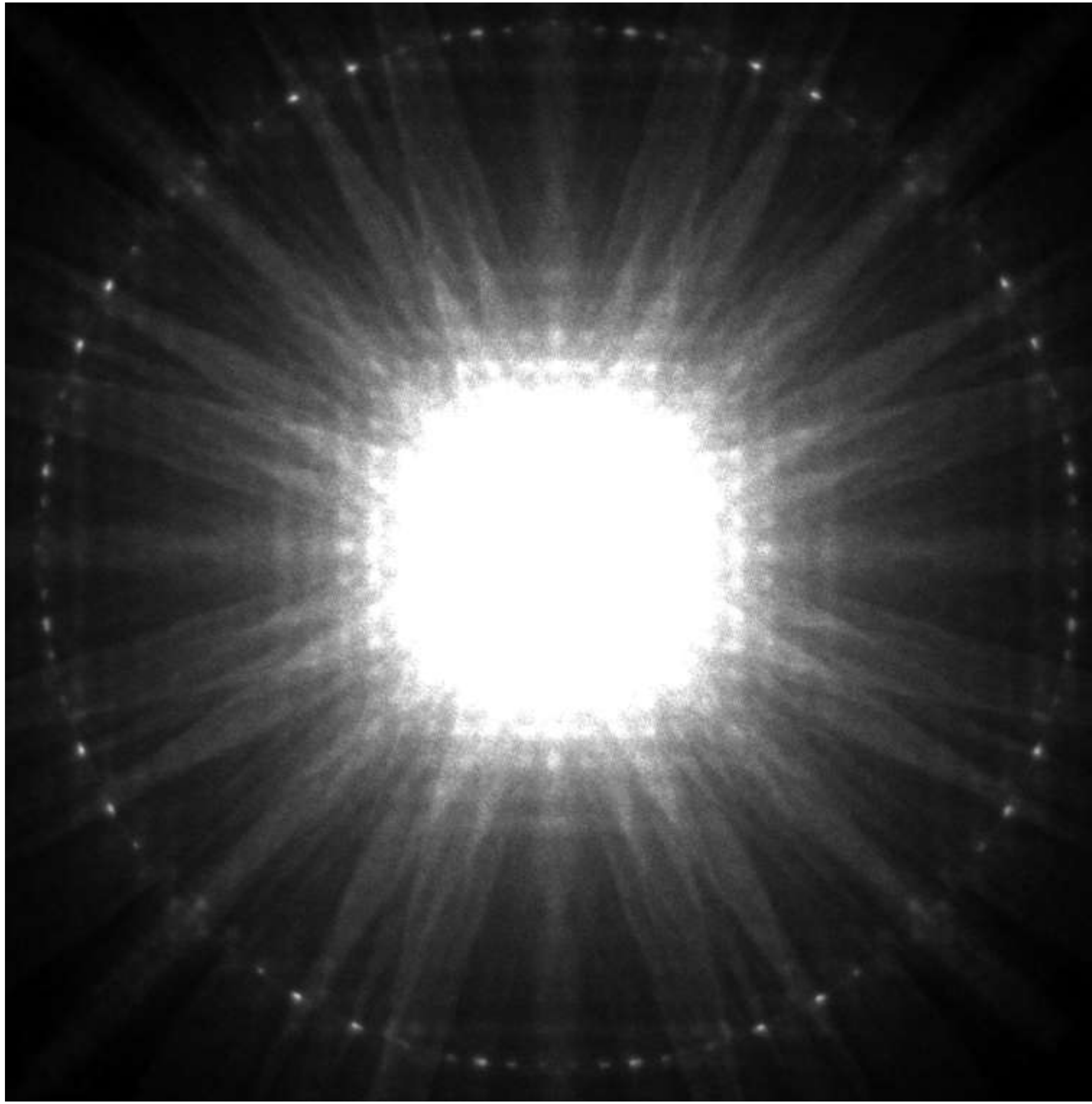
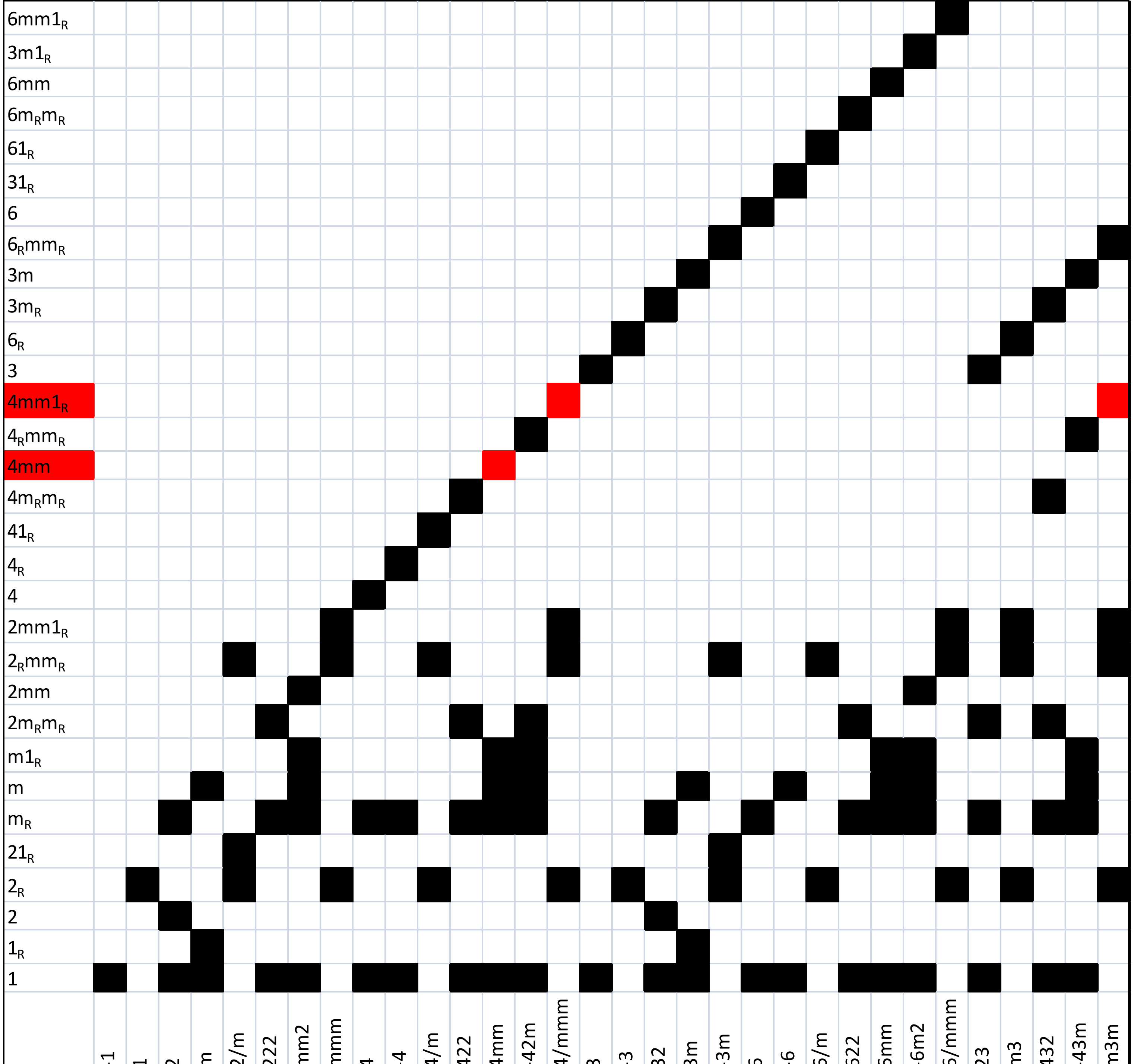


Table 7.1: Diffraction Groups and Pattern Symmetries

diffraction group	bright field	whole pattern	projection diffraction group
1	1	1	1_R
1_R	2	1	1_R
[…]			
4	4	4	41_R
4_R	4	2	41_R
41_R	4	4	41_R
$4m_Rm_R$	4mm	4	$4mm1_R$
4mm	4mm	4mm	$4mm1_R$
4_Rmm_R	4mm	2mm	$4mm1_R$
$4mm1_R$	4mm	4mm	$4mm1_R$

Table 7.2: Projection Diffraction Groups and Pattern Symmetries

projection diffraction group	bright field	whole pattern
1_R	2	1
[…]		
41_R	4	4
$4mm1_R$	4mm	4mm

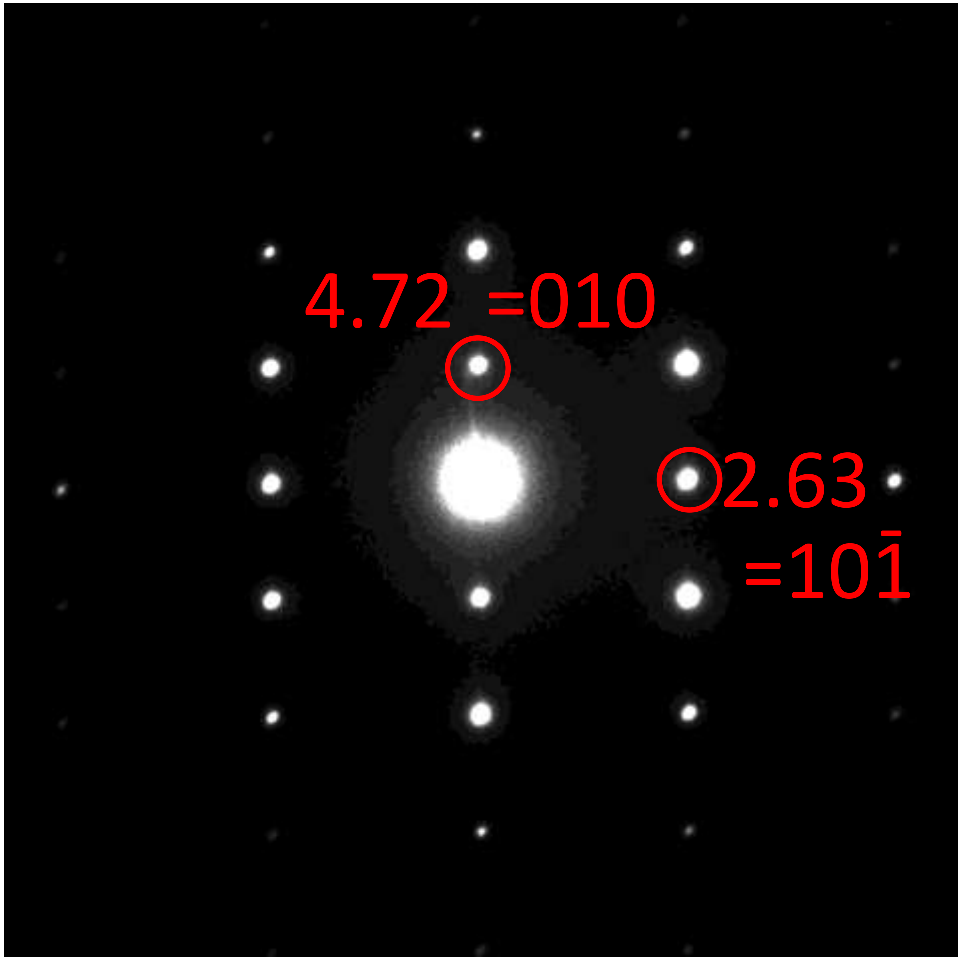

$6mm1_R$
$3m1_R$
6mm
$6m_Rm_R$
61_R
31_R
6
6_Rmm_R
3m
$3m_R$
6_R
3
$4mm1_R$
4_Rmm_R
4mm
$4m_Rm_R$
41_R
4_R
4
$2mm1_R$
2_Rmm_R
2mm
$2m_Rm_R$
$m1_R$
m
m_R
21_R
2_R
2
1_R
1
-1
1
2
m
2/m
222
mm2
mmm
4
-4
4/m
422
4mm
-42m
4/mmm
3
-3
32
3m
-3m
6
-6
6/m
622
6mm
-6m2
6/mmm
23
m3
432
-43m
m3m

Another pattern

Index it.

This is:

- [101] (blue)
- [110] (red)
- [111] (yellow)



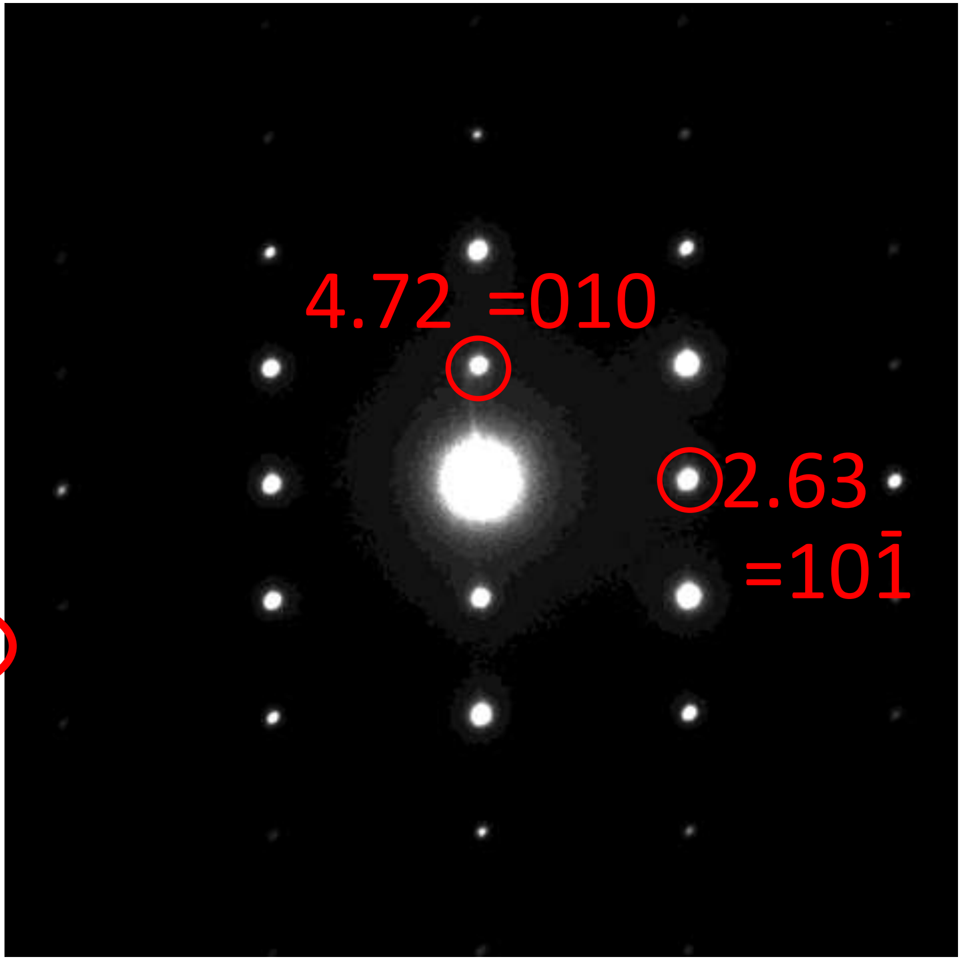
SAED

Another pattern

Index it.

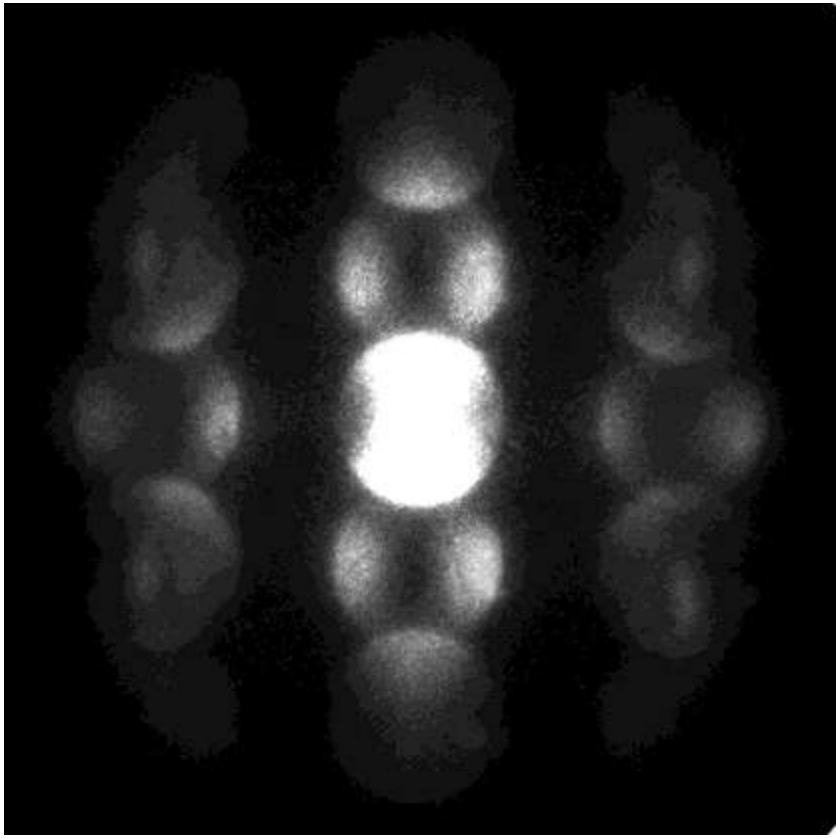
This is:

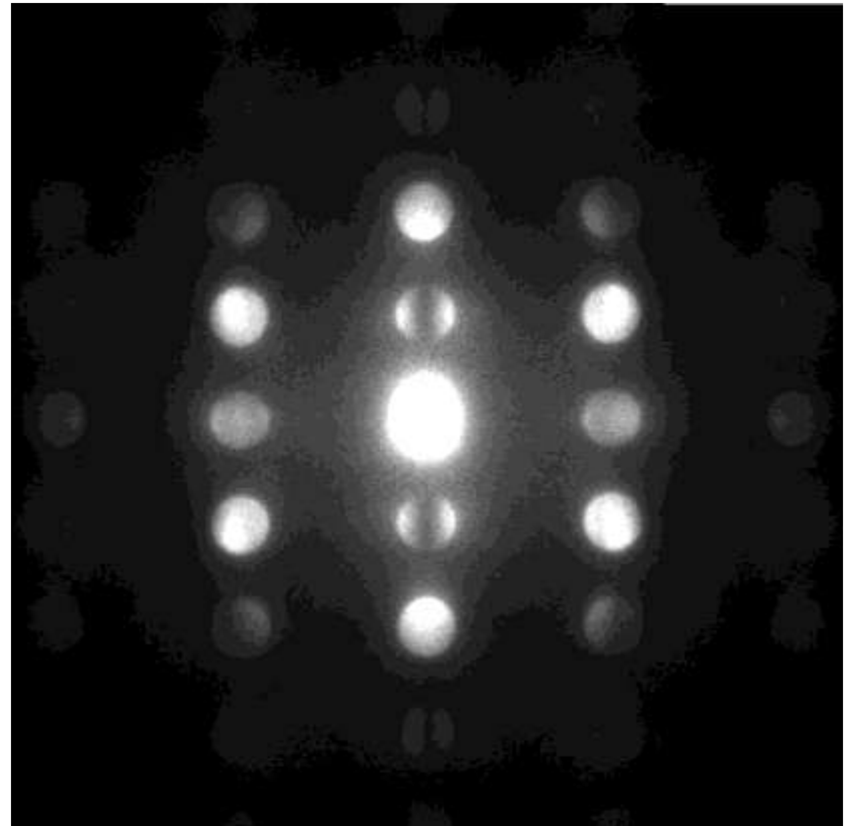
- [101]
- [110]
- [111]



SAED

Projection whole pattern [101]

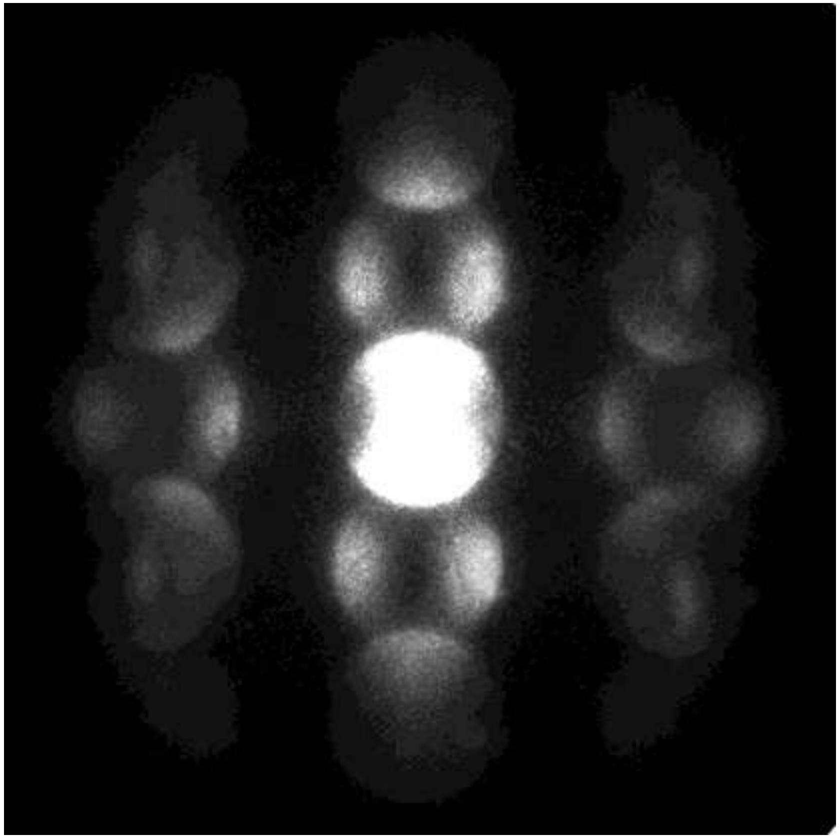


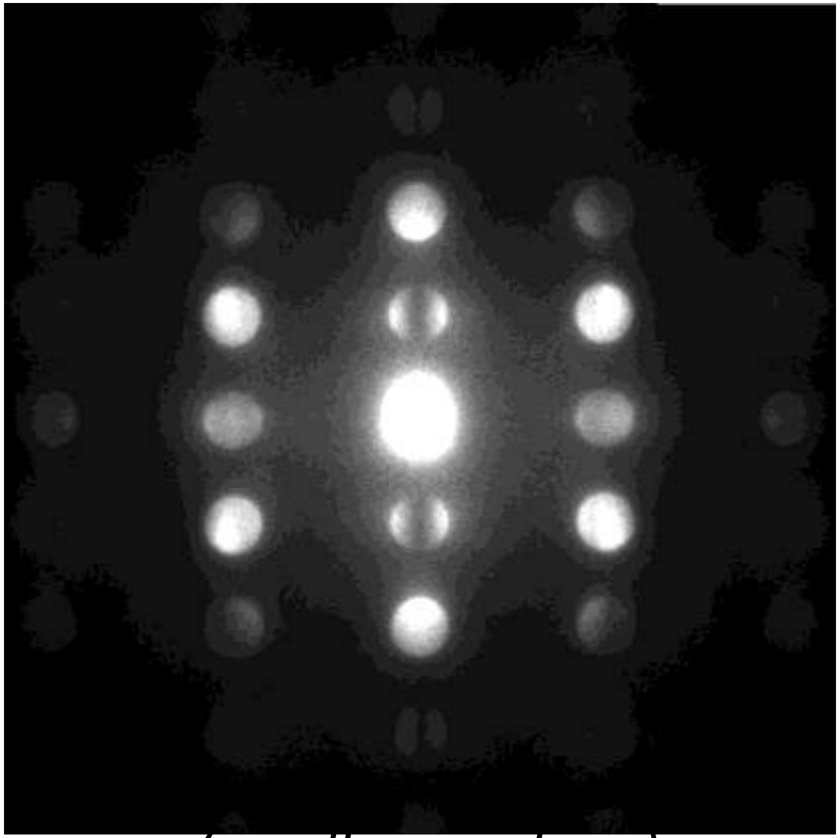


(smaller cond.ap.)

- 2
- m
- 2mm

Projection whole pattern [101]





(smaller cond.ap.)

- 2
- m
- 2mm

Table 7.1: Diffraction Groups and Pattern Symmetries

diffraction group	bright field	whole pattern	projection diffraction group
1	1	1	1_R
1_R	2	1	1_R
2	2	2	21_R
2_R	1	1	21_R
21_R	2	2	21_R
m_R	m	1	$m1_R$
m	m	m	$m1_R$
$m1_R$	2mm	m	$m1_R$
$2m_Rm_R$	2mm	2	$2mm1_R$
2mm	2mm	2mm	$2mm1_R$
2_Rmm_R	m	m	$2mm1_R$
$2mm1_R$	2mm	2mm	$2mm1_R$

Table 7.2: Projection Diffraction Groups and Pattern Symmetries

projection diffraction group	bright field	whole pattern
1_R	2	1
21_R	2	2
$m1_R$	2mm	m
$2mm1_R$	2mm	2mm

Possible projection diffraction group:

- 21_R
- $m1_R$
- $2mm1_R$

Table 7.1: Diffraction Groups and Pattern Symmetries

diffraction group	bright field	whole pattern	projection diffraction group
1	1	1	1_R
1_R	2	1	1_R
2	2	2	21_R
2_R	1	1	21_R
21_R	2	2	21_R
m_R	m	1	$m1_R$
m	m	m	$m1_R$
$m1_R$	2mm	m	$m1_R$
$2m_Rm_R$	2mm	2	$2mm1_R$
2mm	2mm	2mm	$2mm1_R$
2_Rmm_R	m	m	$2mm1_R$
$2mm1_R$	2mm	2mm	$2mm1_R$

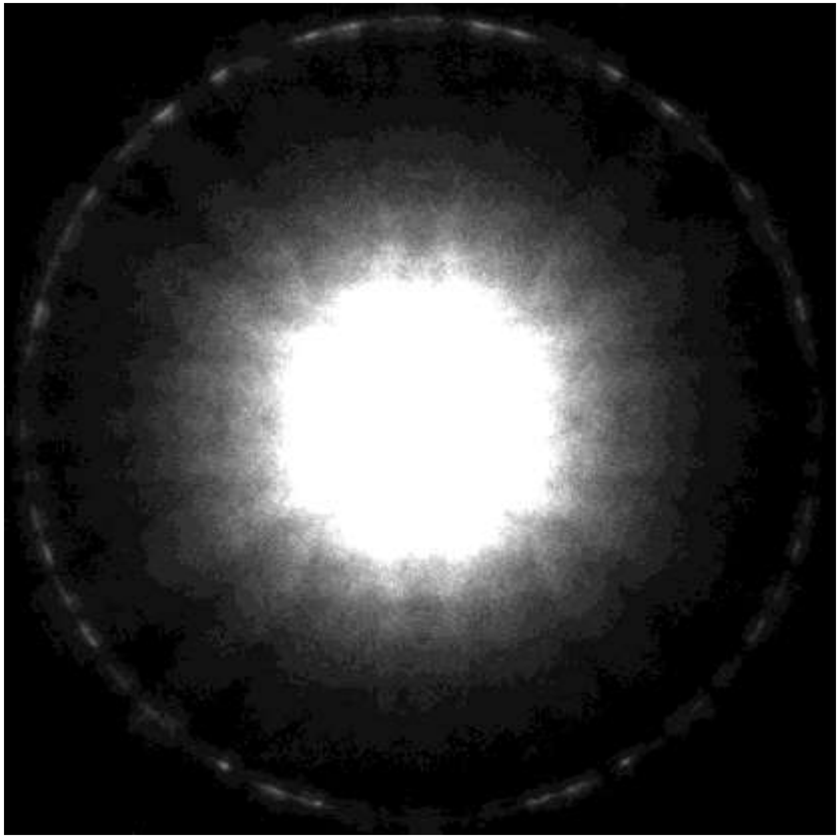
Table 7.2: Projection Diffraction Groups and Pattern Symmetries

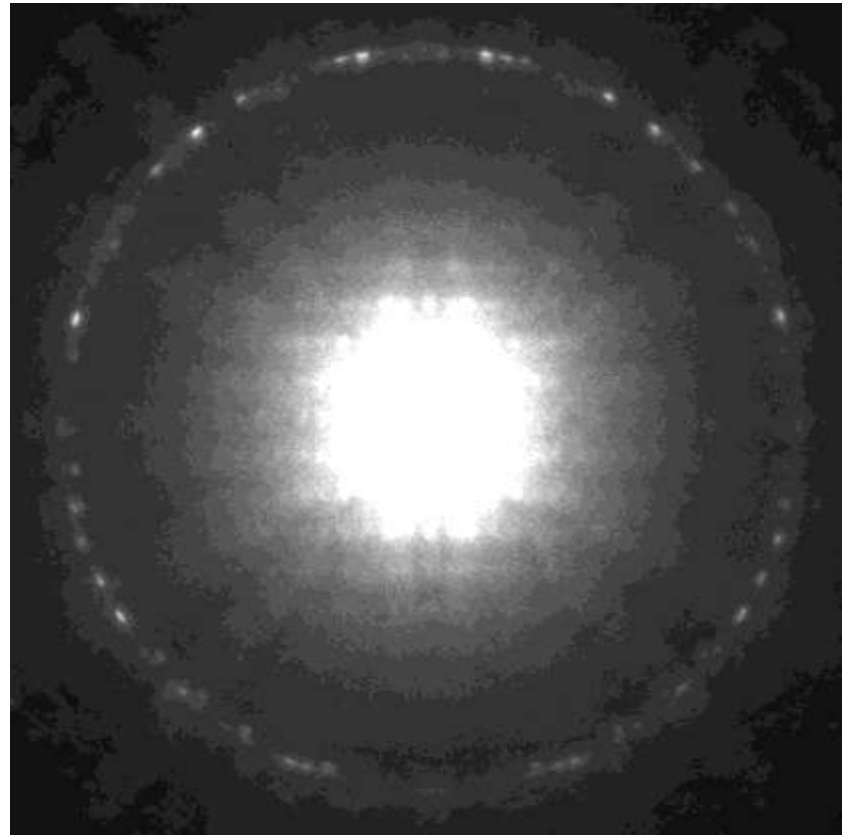
projection diffraction group	bright field	whole pattern
1_R	2	1
21_R	2	2
$m1_R$	2mm	m
$2mm1_R$	2mm	2mm

Possible projection diffraction group:

- 21_R
- $m1_R$
- $2mm1_R$

Whole pattern [101]

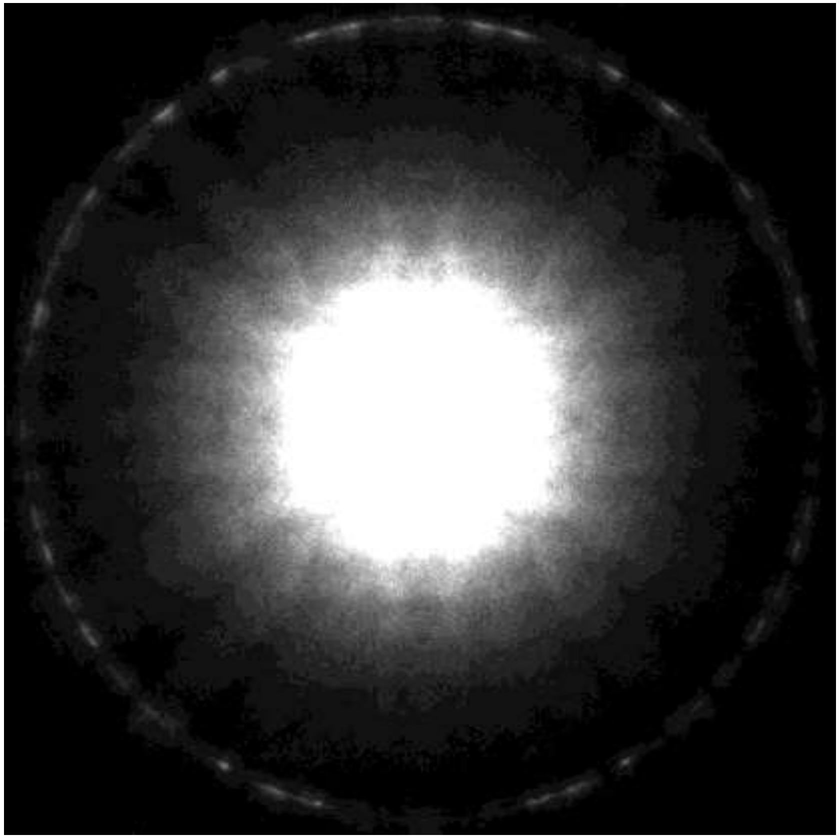


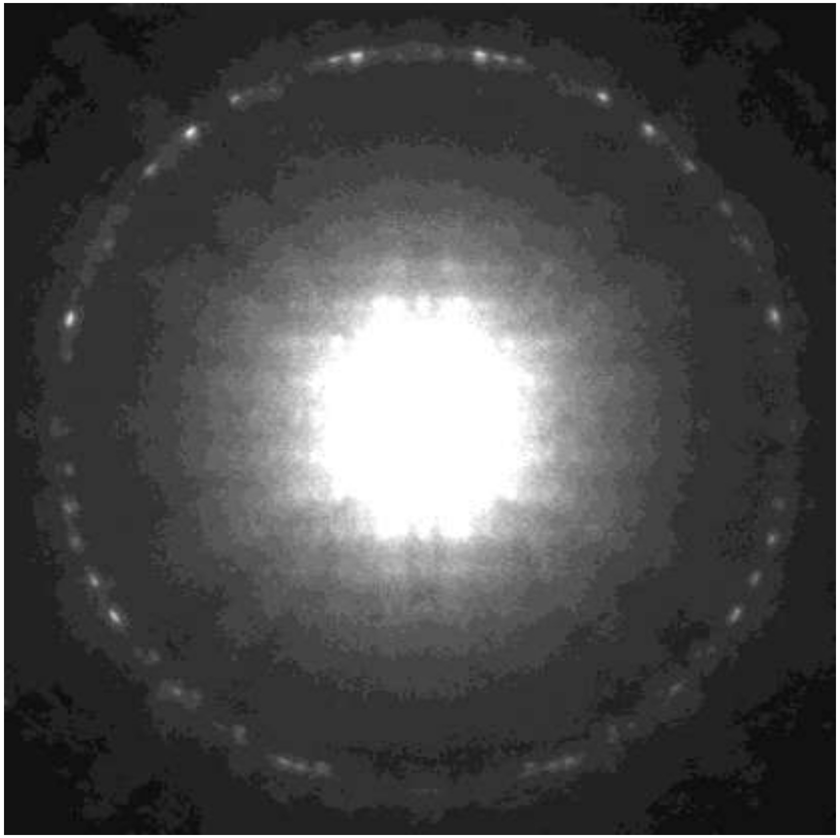


(smaller cond.ap.)

- 2
- m
- 2mm

Whole pattern [101]





(smaller cond.ap.)

- 2
- m
- 2mm

Table 7.1: Diffraction Groups and Pattern Symmetries

diffraction group	bright field	whole pattern	projection diffraction group
1	1	1	1_R
1_R	2	1	1_R
2	2	2	21_R
2_R	1	1	21_R
21_R	2	2	21_R
m_R	m	1	$m1_R$
m	m	m	$m1_R$
$m1_R$	2mm	m	$m1_R$
$2m_Rm_R$	2mm	2	$2mm1_R$
2mm	2mm	2mm	$2mm1_R$
2_Rmm_R	m	m	$2mm1_R$
$2mm1_R$	2mm	2mm	$2mm1_R$

Table 7.2: Projection Diffraction Groups and Pattern Symmetries

projection diffraction group	bright field	whole pattern
1_R	2	1
21_R	2	2
$m1_R$	2mm	m
$2mm1_R$	2mm	2mm

Diffraction group:

- 2mm
- 2_Rmm_R
- $2mm1_R$

Table 7.1: Diffraction Groups and Pattern Symmetries

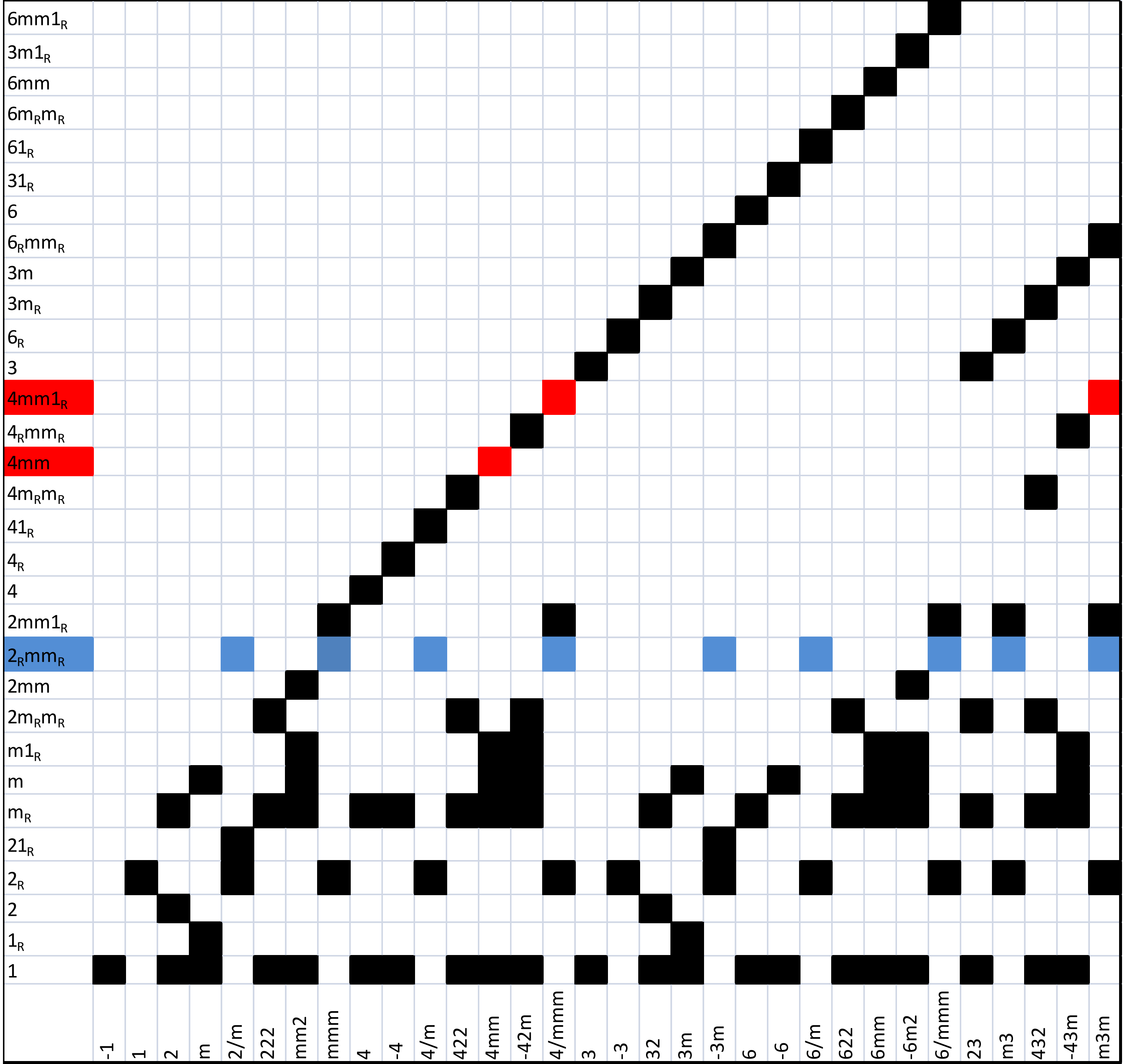
diffraction group	bright field	whole pattern	projection diffraction group
1	1	1	1_R
1_R	2	1	1_R
2	2	2	21_R
2_R	1	1	21_R
21_R	2	2	21_R
m_R	m	1	$m1_R$
m	m	m	$m1_R$
$m1_R$	2mm	m	$m1_R$
$2m_Rm_R$	2mm	2	$2mm1_R$
2mm	2mm	2mm	$2mm1_R$
2_Rmm_R	m	m	$2mm1_R$
$2mm1_R$	2mm	2mm	$2mm1_R$

Table 7.2: Projection Diffraction Groups and Pattern Symmetries

projection diffraction group	bright field	whole pattern
1_R	2	1
21_R	2	2
$m1_R$	2mm	m
$2mm1_R$	2mm	2mm

Diffraction group:

- 2mm
- 2_Rmm_R
- $2mm1_R$


$6mm1_R$
$3m1_R$
6mm
$6m_Rm_R$
61_R
31_R
6
6_Rmm_R
3m
$3m_R$
6_R
3
$4mm1_R$
4_Rmm_R
4mm
$4m_Rm_R$
41_R
4_R
4
$2mm1_R$
2_Rmm_R
2mm
$2m_Rm_R$
$m1_R$
m
m_R
21_R
2_R
2
1_R
1
-1
1
2
m
2/m
222
mm2
mmm
4
-4
4/m
422
4mm
-42m
4/mmm
3
-3
32
3m
-3m
6
-6
6/m
622
6mm
-6m2
6/mmm
23
m3
432
-43m
m3m

Possible point groups

4/mmm

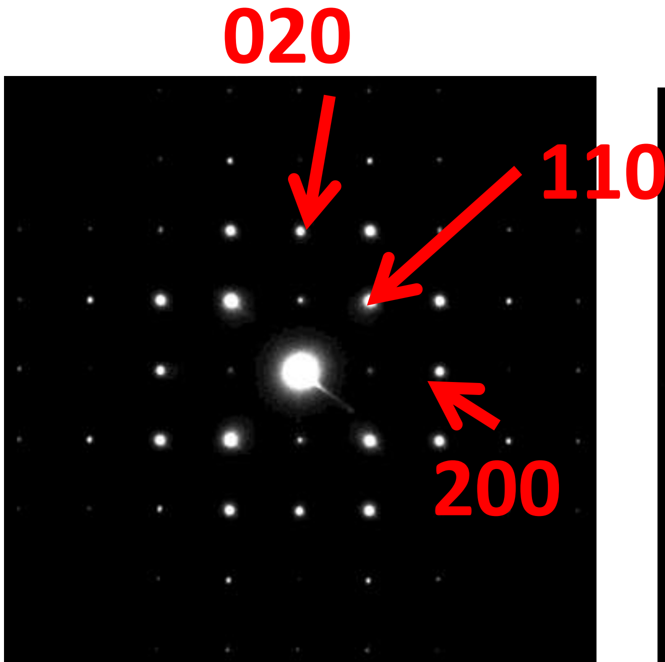
~~m3m~~

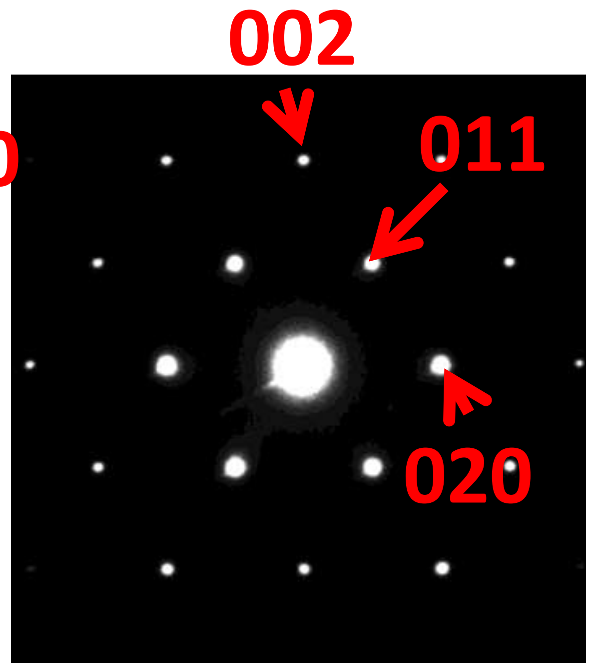
CBED

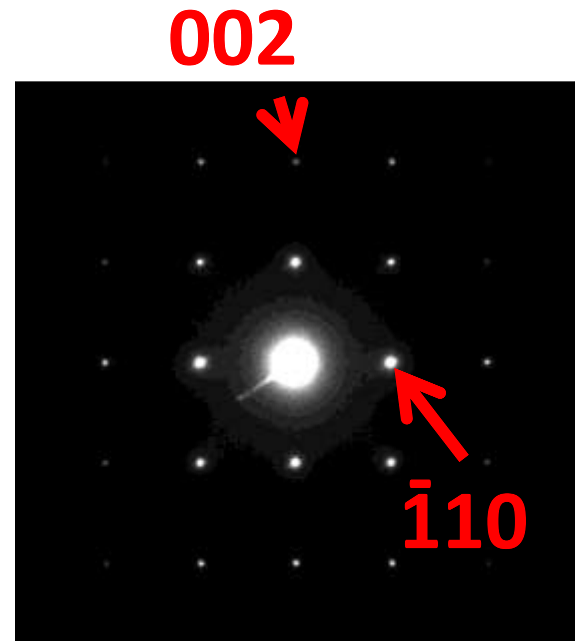
Reflection conditions							Extinction symbol	Laue class 4/m			Laue class 4/mmm (4/m 2/m 2/m)			
								Point group						
hkl	hk0	0kl	hhl	00l	0k0	hh0		4	$\bar{4}$	4/m	422	4mm	$\bar{4}2m$ $\bar{4}m2$	4/mmm
							$P - - -$	$P4$ (75)	$P\bar{4}$ (81)	$P4/m$ (83)	$P422$ (89)	$P4mm$ (99)	$P\bar{4}2m$ (111)	$P4/mmm$ (123)
													$P\bar{4}m2$ (115)	
					k		$P-2_1-$				$P42_12$ (90)		$P\bar{4}2_1m$ (113)	
				l			$P4_2- -$	$P4_2$ (77)		$P4_2/m$ (84)	$P4_222$ (93)			
				l	k		$P4_22_1-$				$P4_22_12$ (94)			
				$l = 4n$			$P4_1- -$	$\{P4_1$ (76), $P4_3$ (78)$\}$†			$\{P4_122$ (91), $P4_322$ (95)$\}$†			
				$l = 4n$	k		$P4_12_1-$				$\{P4_12_12$ (92), $P4_32_12$ (96)$\}$†			
			l	l			$P - - c$					$P4_2mc$ (105)	$P\bar{4}2c$ (112)	$P4_2/mmc$ (131)
			l	l	k		$P-2_1c$						$P\bar{4}2_1c$ (114)	
		k			k		$P - b -$					$P4bm$ (100)	$P\bar{4}b2$ (117)	$P4/mbm$ (127)
		k	l	l	k		$P - bc$					$P4_2bc$ (106)		$P4_2/mbc$ (135)
		l		l			$P - c -$					$P4_2cm$ (101)	$P\bar{4}c2$ (116)	$P4_2/mcm$ (132)
		l	l	l			$P - cc$					$P4cc$ (103)		$P4/mcc$ (124)
		$k+l$		l	k		$P - n -$					$P4_2nm$ (102)	$P\bar{4}n2$ (118)	$P4_2/mnm$ (136)
		$k+l$	l	l	k		$P - nc$					$P4nc$ (104)		$P4/mnc$ (128)
	$h+k$				k		$Pn - -$			$P4/n$ (85)				$P4/nmm$ (129)
	$h+k$			l	k		$P4_2/n- -$			$P4_2/n$ (86)				
	$h+k$		l	l	k		$Pn - c$							$P4_2/nmc$ (137)

from: International Tables for Crystallography Volume A, ed. Theo Hahn, Kluwer Ac. Pub., 2002

Combine with information about reflection conditions from SAED patterns



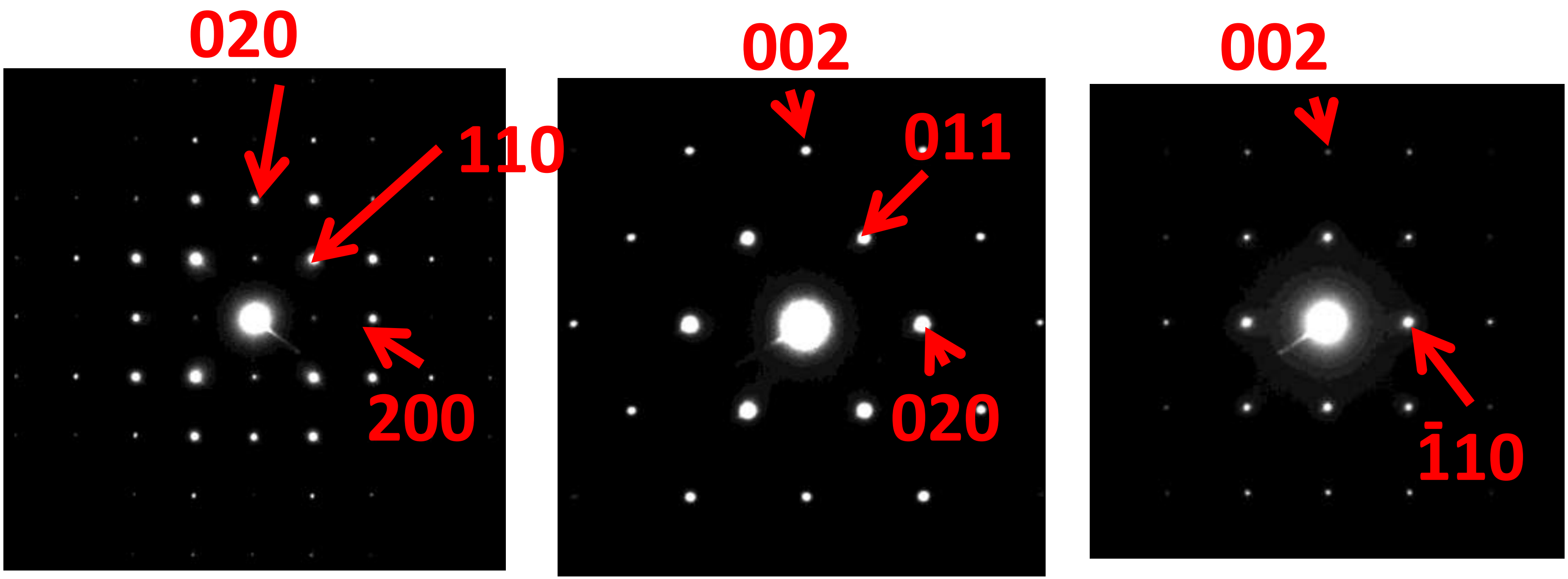




hkl:

- no conditions
- h+k+l=2n

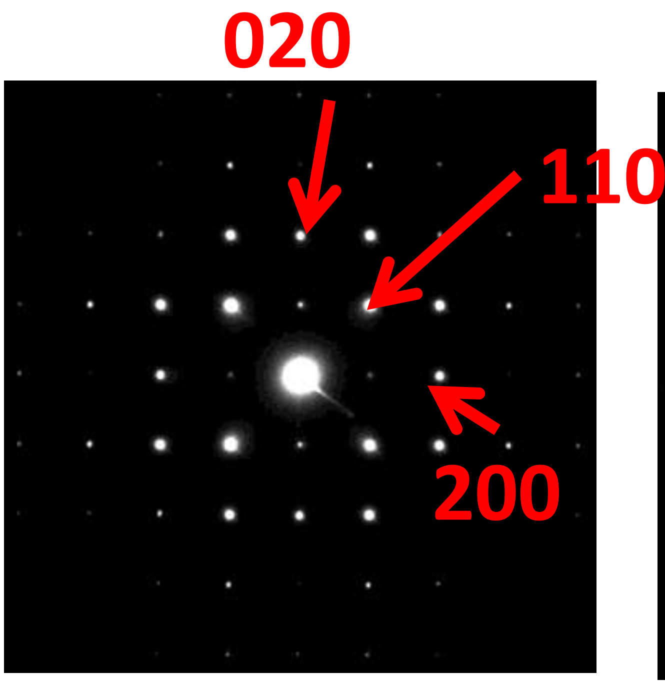
Combine with information about reflection conditions from SAED patterns



hkl:

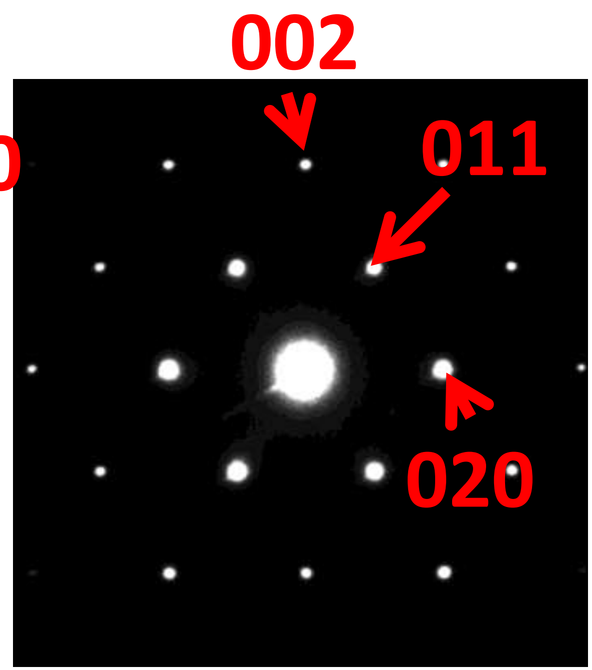
- no conditions
- h+k+l=2n

Combine with information about reflection conditions from SAED patterns



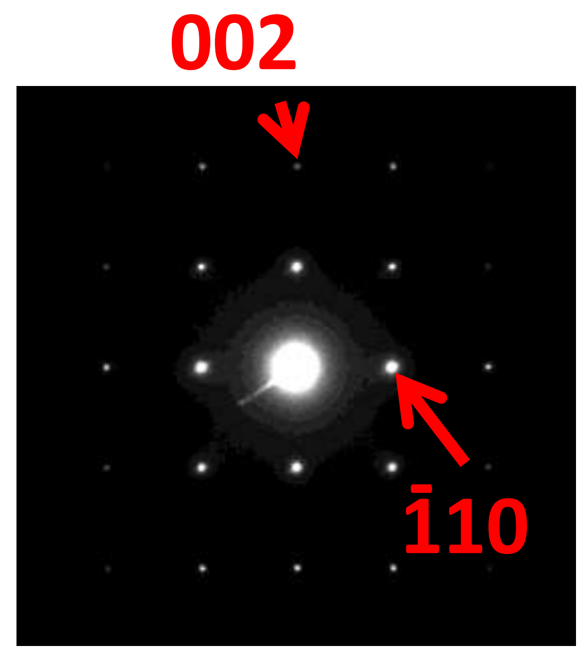
hk0:

- no conditions
- h+k=2n



0kl:

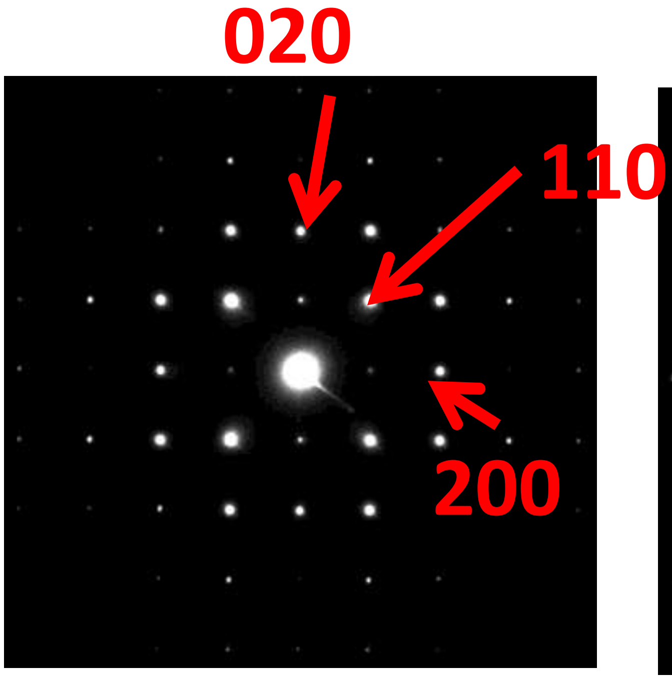
- no conditions
- k+l=2n
- k=2n or l=2n

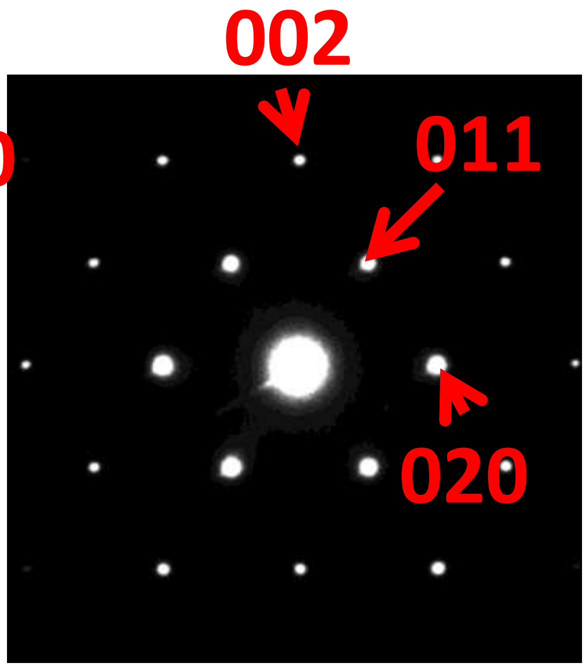


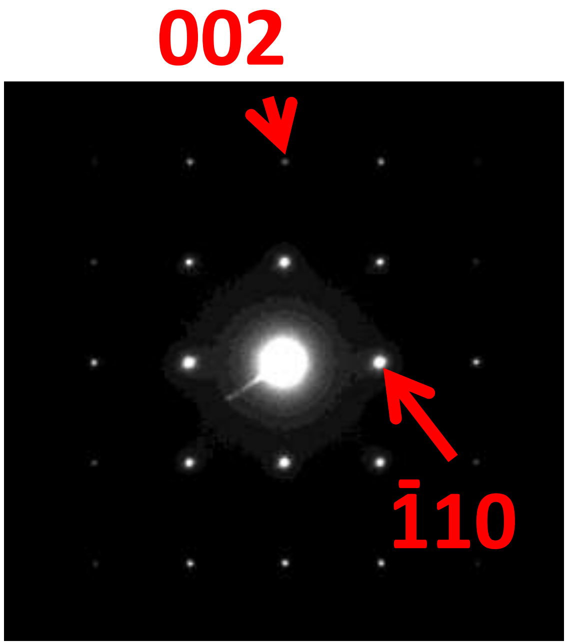
hhl:

- no conditions
- l=2n

Combine with information about reflection conditions from SAED patterns





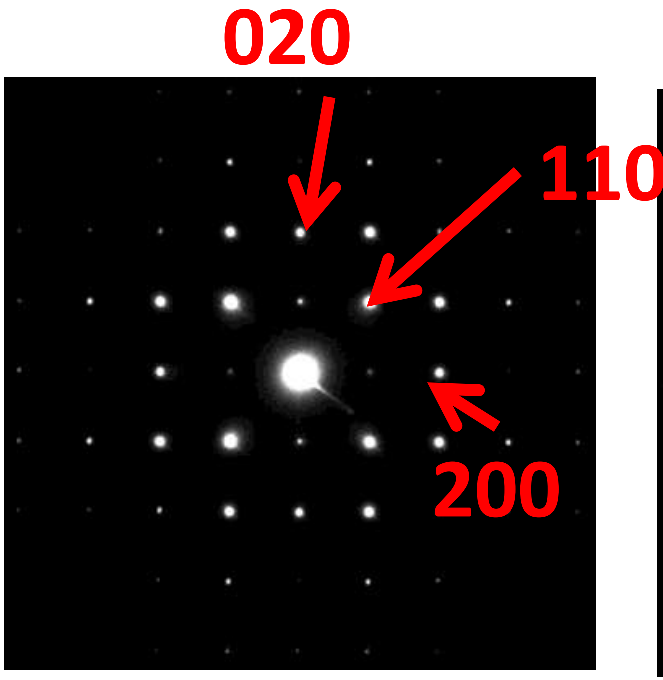


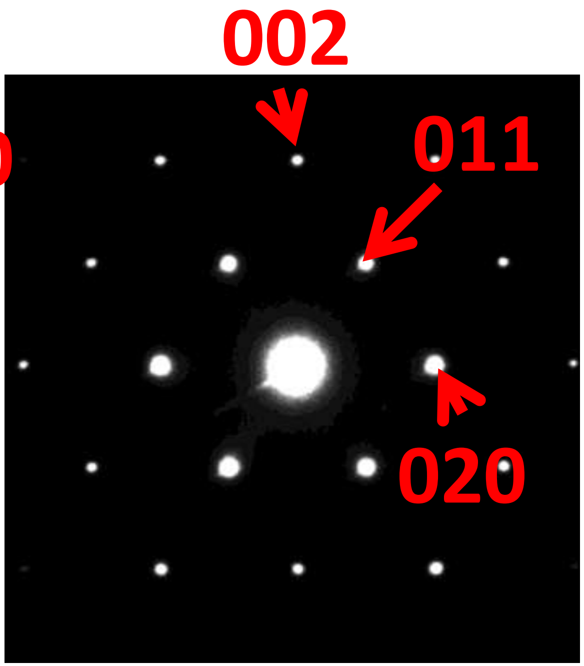
hk0:
- no conditions
- h+k=2n

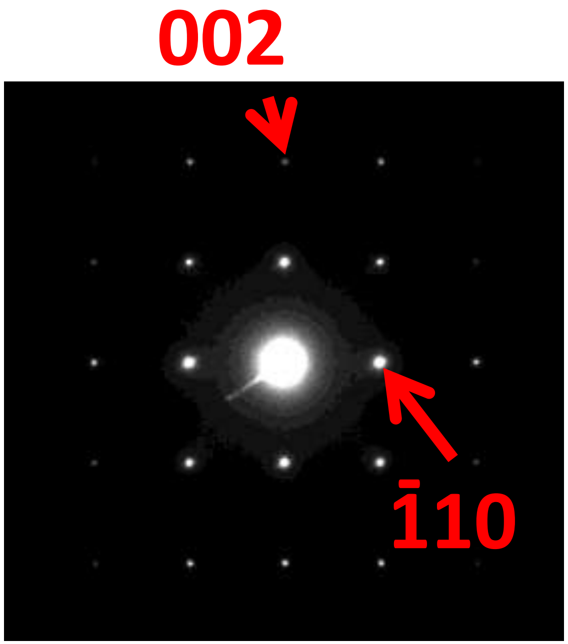
0kl:
- no conditions
- k+l=2n
- k=2n or l=2n

hhl:
- no conditions
- l=2n

Combine with information about reflection conditions from SAED patterns







hk0:

- no conditions
- h+k=2n

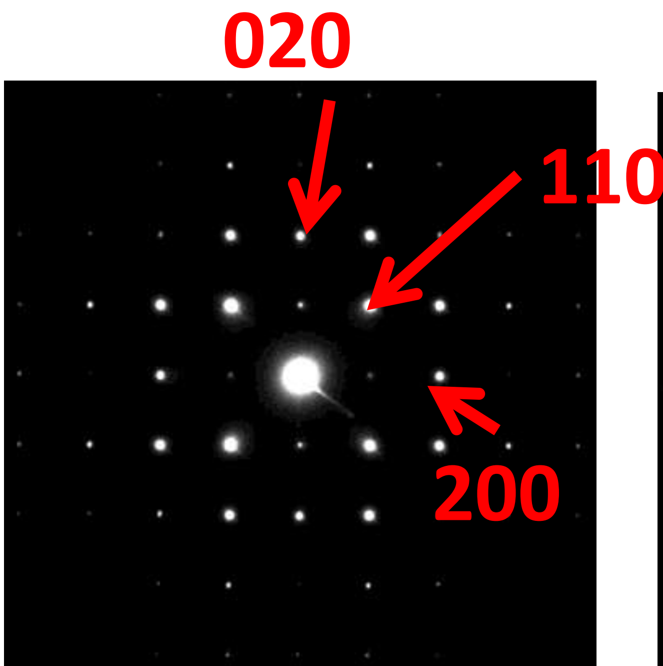
0kl:

- no conditions
- k+l=2n
- k=2n or l=2n

hhl:

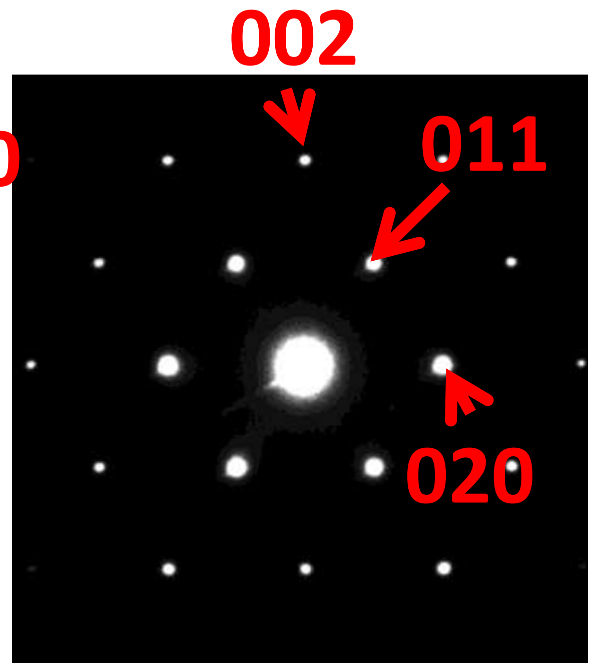
- no conditions
- l=2n

Combine with information about reflection conditions from SAED patterns



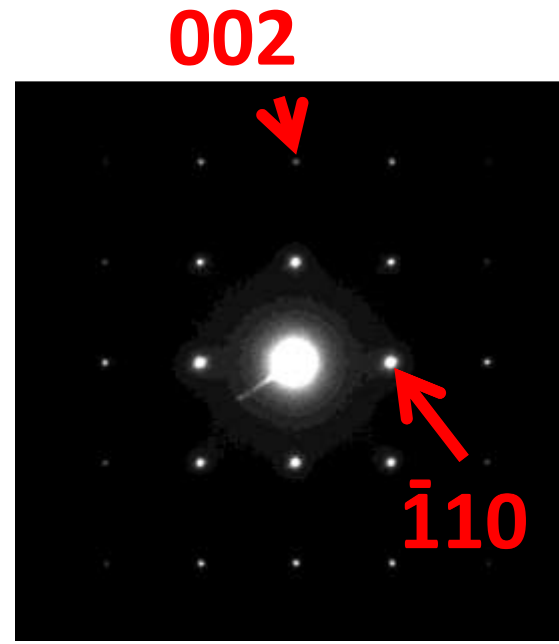
hk0:

- no conditions
- h+k=2n



0kl:

- no conditions
- k+l=2n
- k=2n or l=2n



hhl:

- no conditions
- l=2n

International Tables

Reflection conditions							Extinction symbol	Laue class						
								4/m			4/mmm (4/m 2/m 2/m)			
								Point group						
hkl	$hk0$	$0kl$	hhl	$00l$	$0k0$	$hh0$	symbol	4	$\bar{4}$	$4/m$	422	$4mm$	$\bar{4}2m$ $\bar{4}m2$	$4/mmm$
							$P - - -$	$P4$ (75)	$P\bar{4}$ (81)	$P4/m$ (83)	$P422$ (89)	$P4mm$ (99)	$P\bar{4}2m$ (111)	[illegible] (123)
													$P\bar{4}m2$ (115)	
					k		$P-2_1-$				$P42_12$ (90)		$P\bar{4}2_1m$ (113)	
				l			$P4_2--$	$P4_2$ (77)		$P4_2/m$ (84)	$P4_222$ (93)			
				l	k		$P4_22_1-$				$P4_22_12$ (94)			
				$l=4n$			$P4_1--$	{$P4_1$ (76), $P4_3$ (78)}†			{$P4_122$ (91), $P4_322$ (95)}†			
				$l=4n$	k		$P4_12_1-$				{$P4_12_12$ (92), $P4_32_12$ (96)}†			
			l	l			$P--c$					$P4_2mc$ (105)	$P\bar{4}2c$ (112)	$P4_2/$[illegible]mc (131)
			l	l	k		$P-2_1c$						$P\bar{4}2_1c$ (114)	
		k			k		$P-b-$					$P4bm$ (100)	$P\bar{4}b2$ (117)	$P4/$[illegible]m (127)
		k	l	l	k		$P-bc$					$P4_2bc$ (106)		$P4_2/$[illegible]bc (135)
		l		l			$P-c-$					$P4_2cm$ (101)	$P\bar{4}c2$ (116)	$P4_2/$[illegible]cm (132)
		l	l	l			$P-cc$					$P4cc$ (103)		$P4/$[illegible] (124)
		$k+l$		l	k		$P-n-$					[illegible]	[illegible]	$P4_2/mnm$ (136)
		$k+l$	l	l	k		$P-nc$					$P4nc$ (104)		[illegible]
	$h+k$				k		$Pn--$			$P4/n$ (85)				$P4/nmm$ (129)
	$h+k$			l	k		$P4_2/n--$			$P4_2/n$ (86)				
	$h+k$		l	l	k		$Pn-c$							$P4_2/nmc$ (137)

CBED

SAED

Space Group $P4_2/mnm$

3. Precession electron diffraction (PED)

Ab initio solution of structures using electron diffraction:

You have as experimental data: only electron diffraction patterns

→

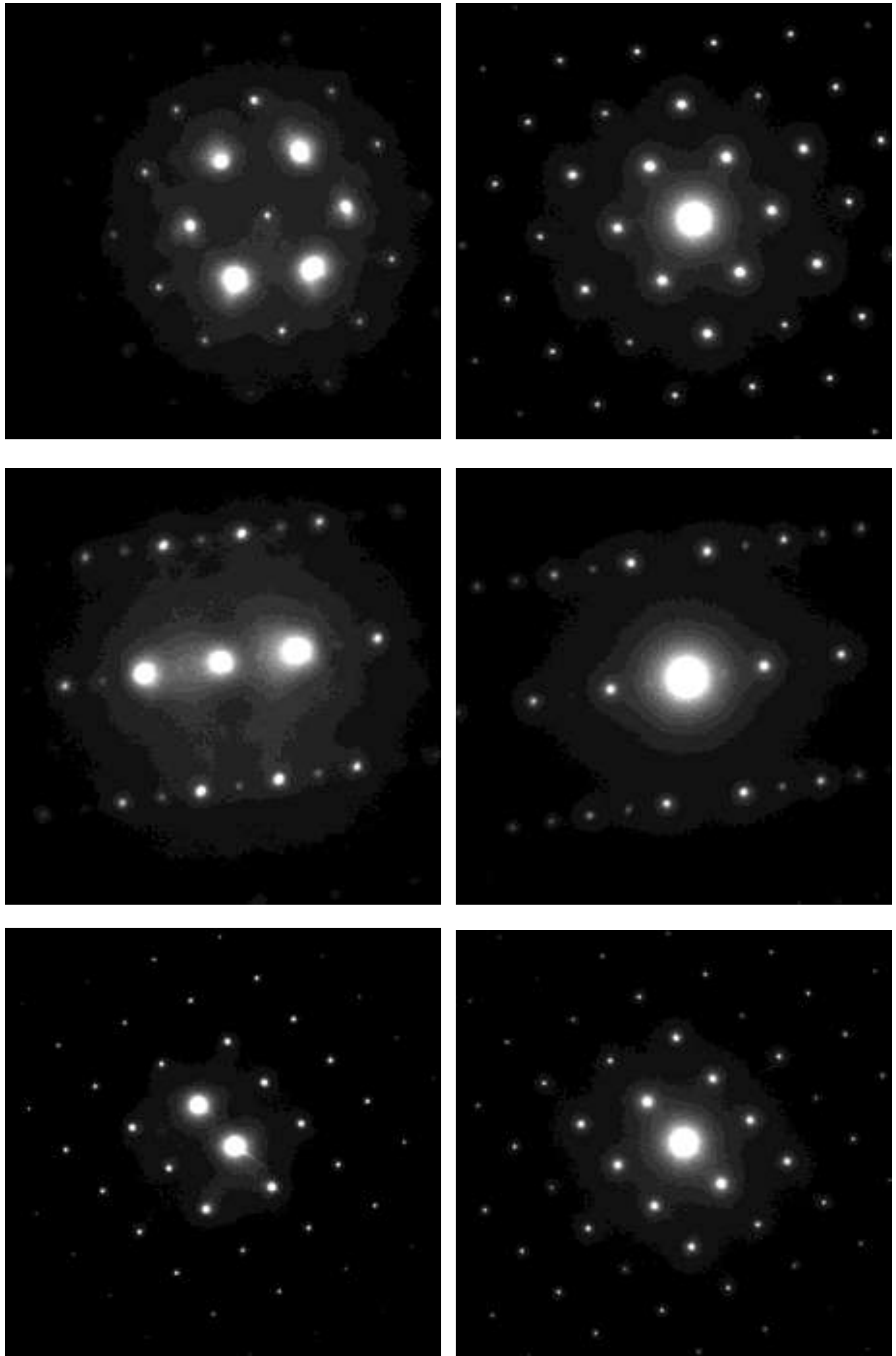
You get: the structure

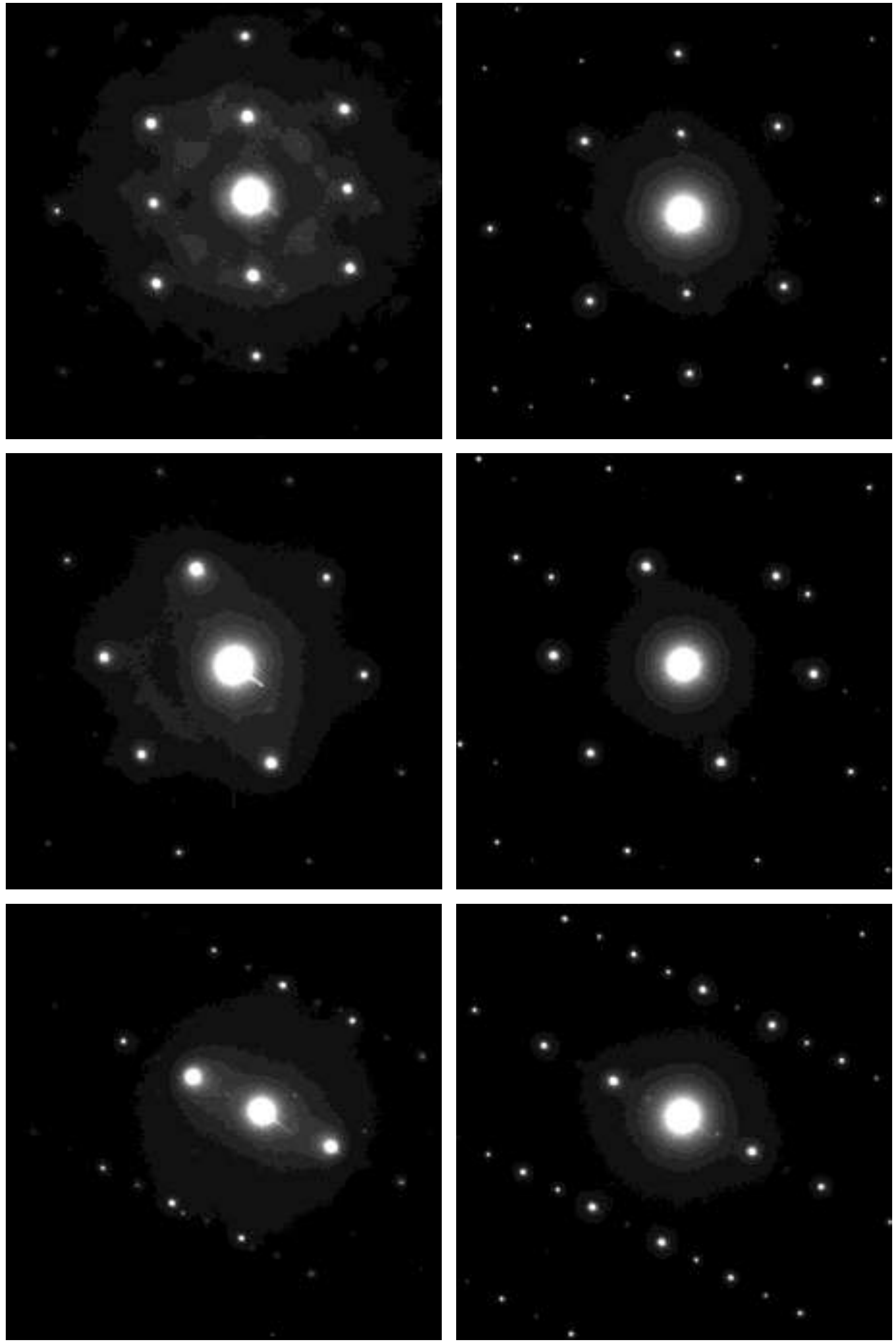
Trouble: dynamical diffraction

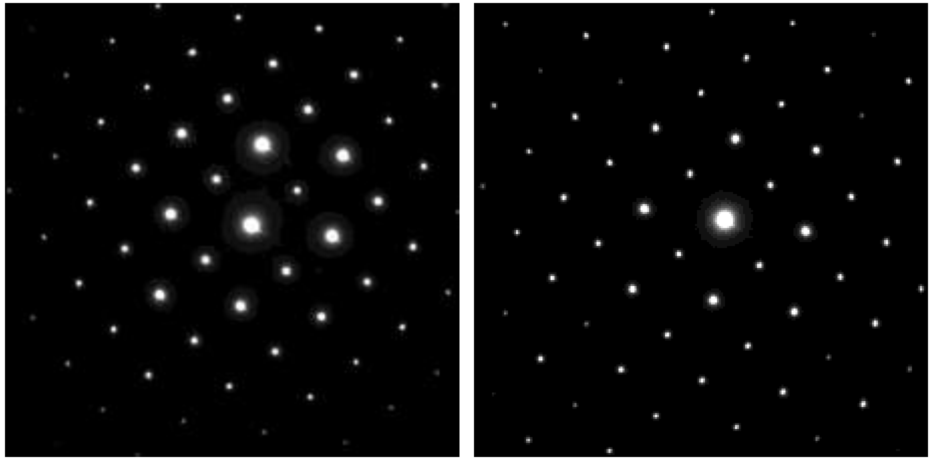
⇨ Precession electron diffraction

Example: SnO_2

Demonstration of the precession technique with EMAP







Intensities of the reflections
from several zones
+
cell parameters and space
group from SAED-CBED
+
composition from EDX/EELS
or nominal composition

STRUCTURE

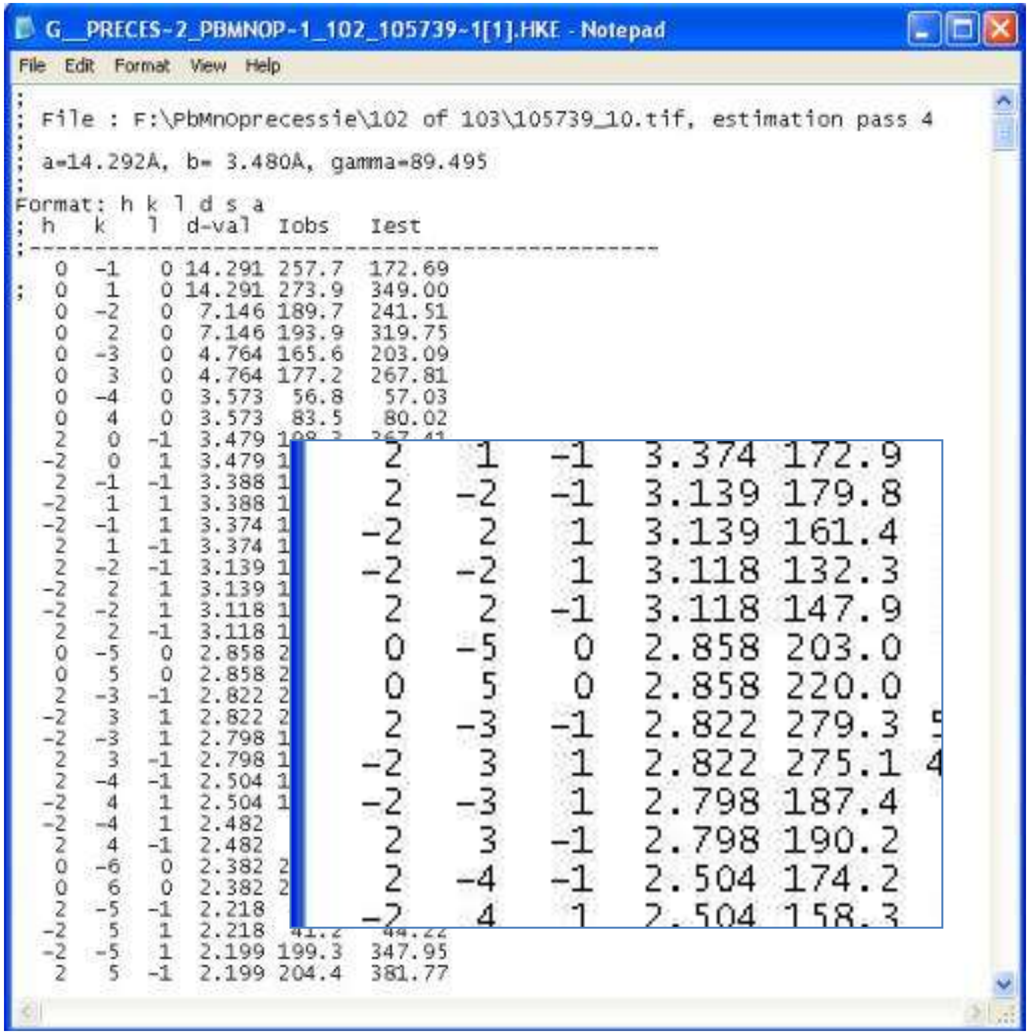
Extract the intensities using

[EDM]

[EXTRAX]

[CRISP]

...



Possibilities to introduce mistakes:

not well oriented

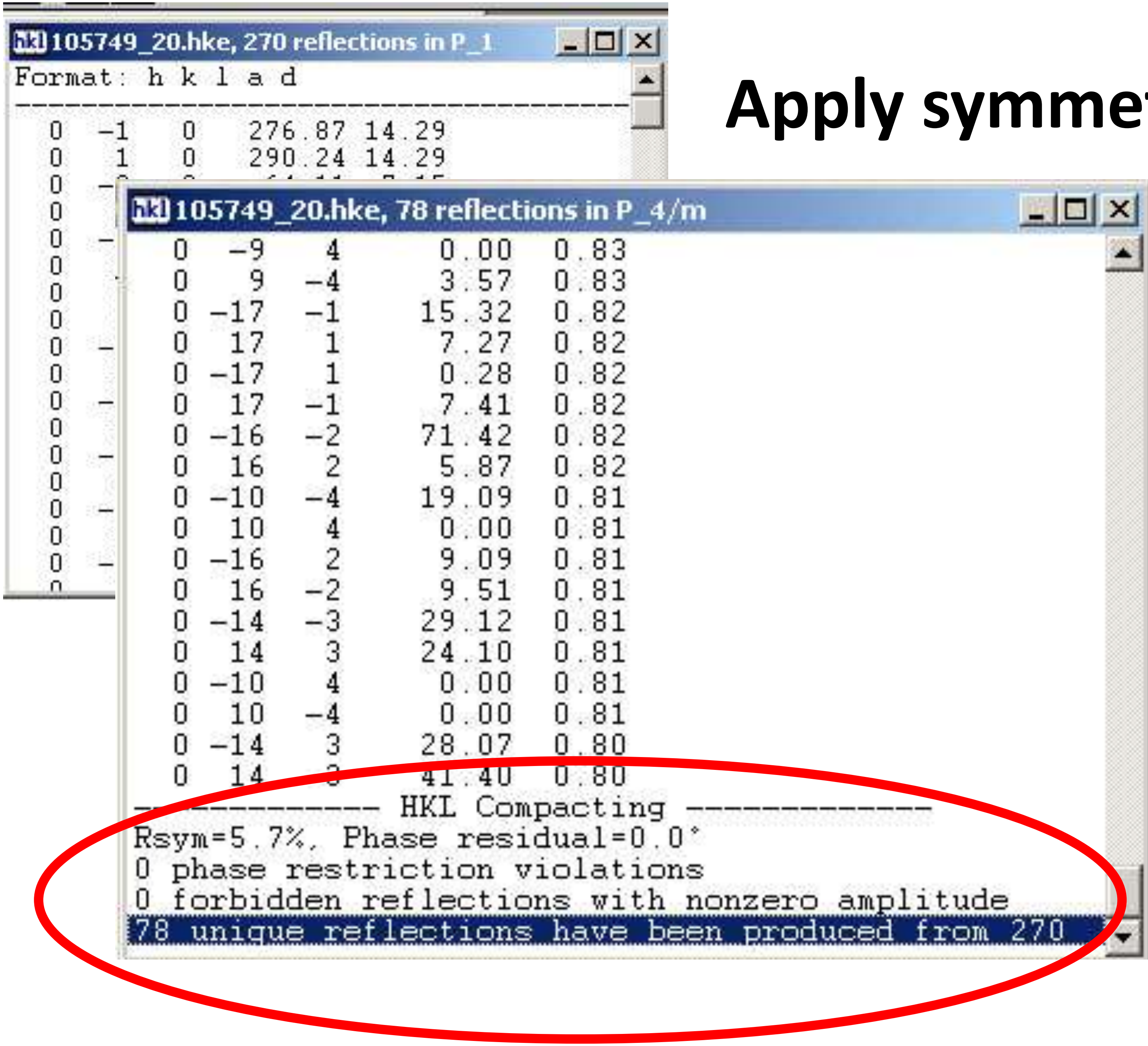
too thick

too small precession angle

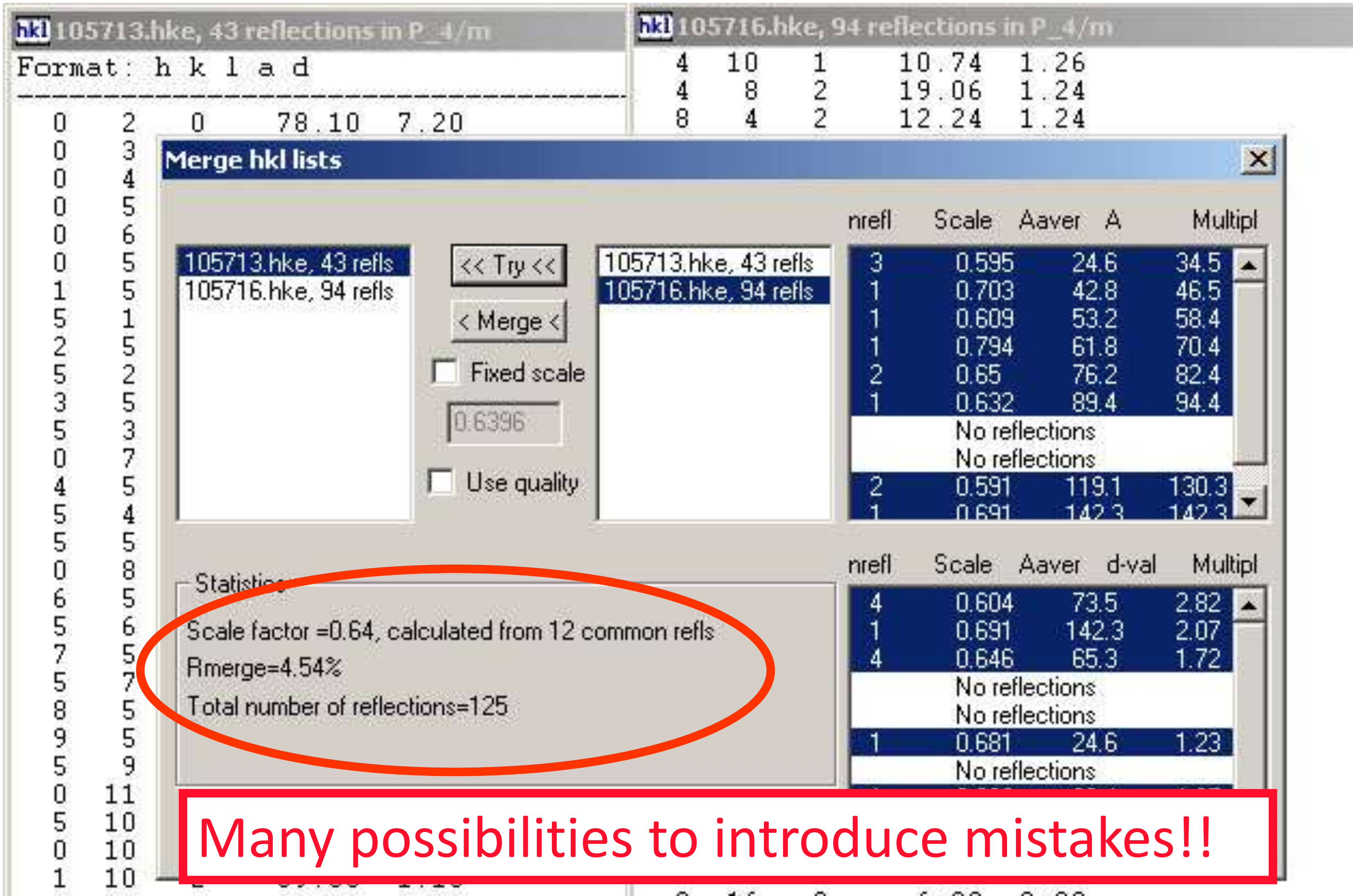
too large precession angle

...

Apply symmetry



Combine separate lists



Many possibilities to introduce mistakes!!

⇨ Direct methods, or optimisation methods made for single crystal data

SIR2008
Fox
Endeavour
…

Right structure càn come out (GIGO).

Purpose of this lecture

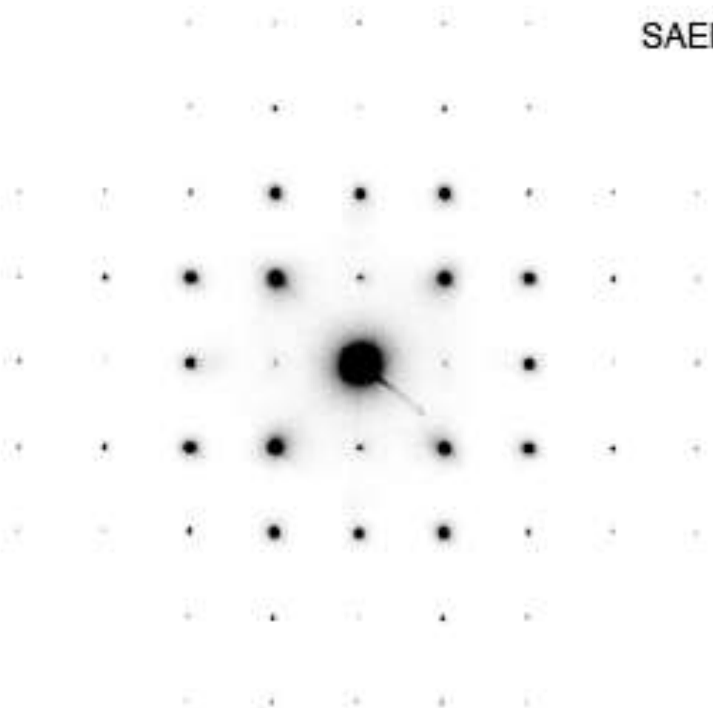
At the end of this lecture, you should be able to

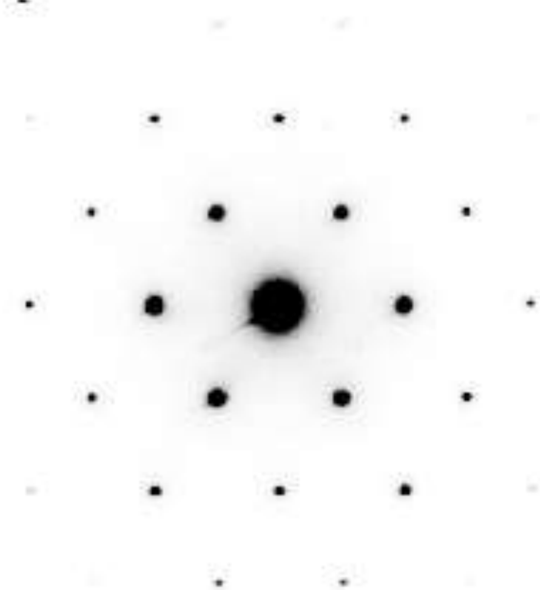
1) index SAED patterns if the cell parameters are known
2) know how to determine unknown cell parameters from SAED patterns
3) determine the possible space groups from SAED patterns
4) determine possible point groups from CBED patterns
5) determine a simple structure ab initio from PED patterns

ED patterns for the exercises

These ED are the same as those on the previous slides, but the contrast has been reversed to enable easy writing.

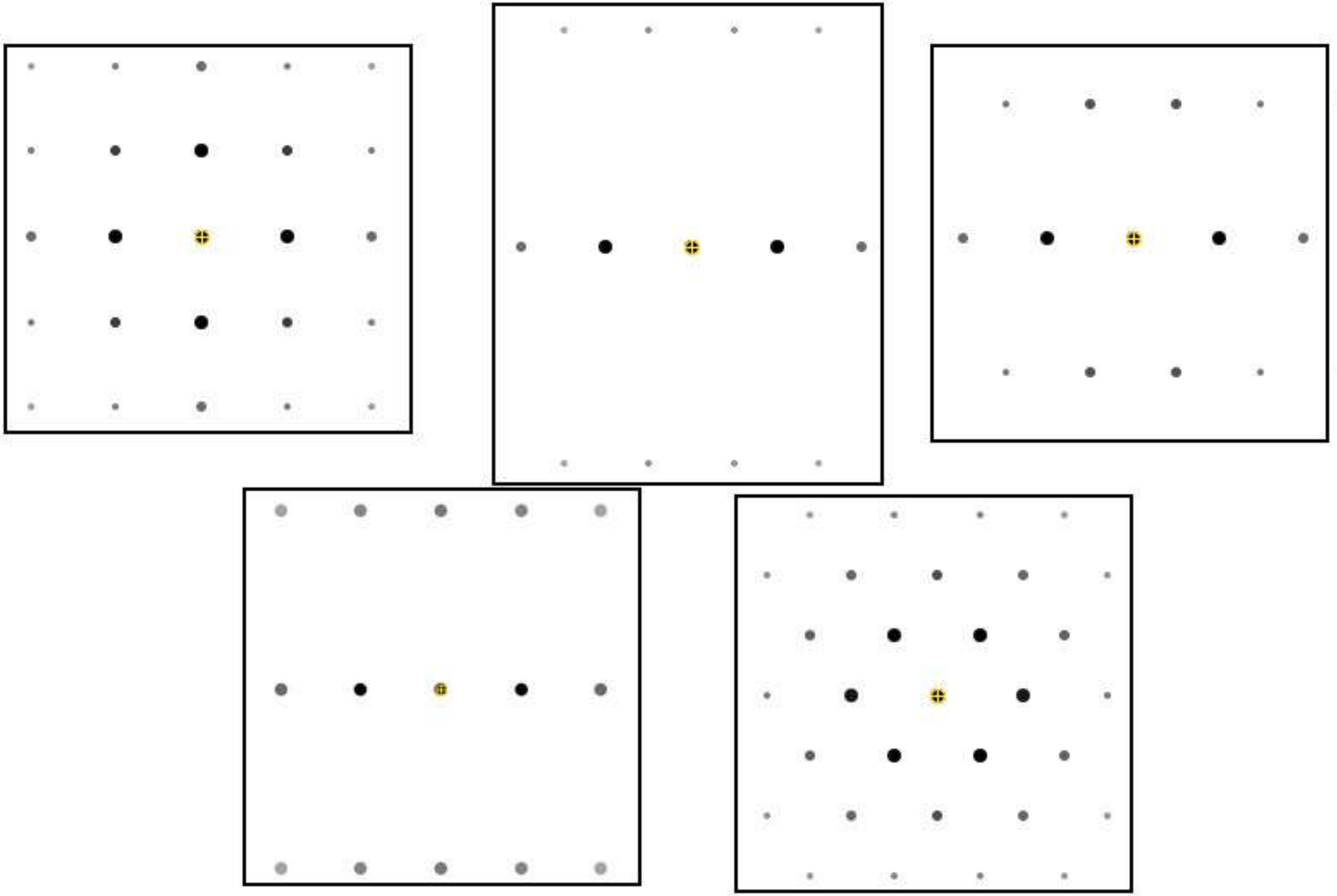
SAED SnO_2



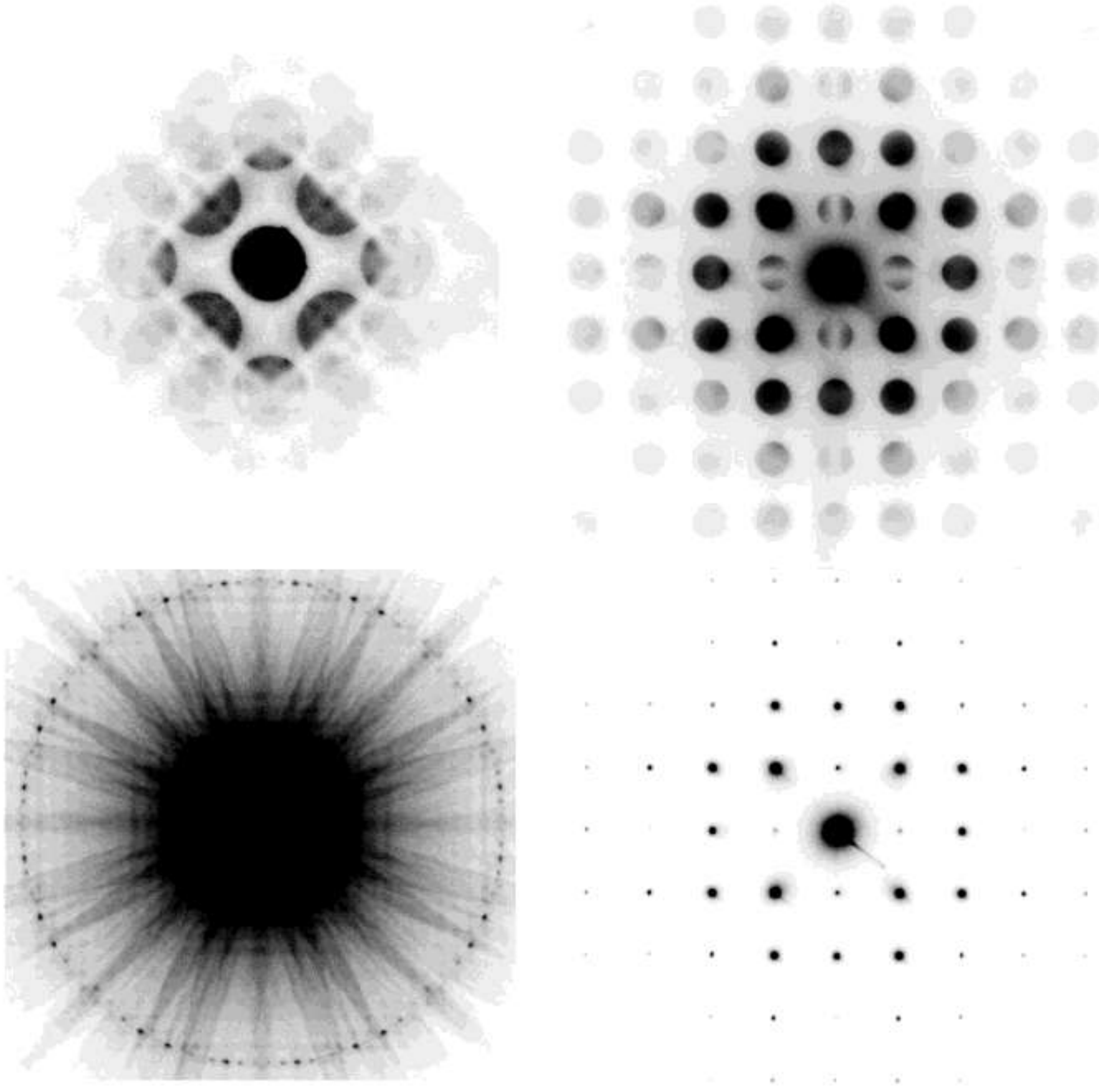


H	K	L	2Theta	d/Å
1	1	0	26.688	3.33754
1	0	1	34.041	2.63158
2	0	0	38.101	2.36000
1	1	1	39.161	2.29848
2	1	0	42.806	2.11085
2	1	1	52.007	1.75697
2	2	0	54.980	1.66877
0	0	2	58.155	1.58500
3	1	0	62.139	1.49260
2	2	1	62.886	1.47666
1	1	2	65.097	1.43175
3	0	1	66.266	1.40930
3	1	1	69.560	1.35039

Calculated SAED Aluminum



CBED and SAED SnO_2 [001]



SAED and CBED SnO_2 second zone